# **EAST Search History**

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	551500	phenyl	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L2	2479	hexenoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L3	40	L2 near5 L1	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L4	176	(562/491).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L5	1461	(514/562).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L6	601	(514/564).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L7	1167	(514/570).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L8	361	(514/571).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L9	241	(562/495).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L10	654	(514/559).CCLS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:53
L11	4257	L4 or L9 or L10 or L5 or L6 or L7 or L8	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53

### **EAST Search History**

					,	
L12	1	L3 and L11	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L13	164286	cyclohexyl	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L14	17	L3 and L13 .	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:53
L15	11	("4513005").URPN.	USPAT	OR	ON	2007/12/11 07:53
L16	0	"49047735"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:54
L17	0	("49047735").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 07:55
L18	82	heptatrienoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 07:56
L19	23	l1 near20 l18	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:02
L20	666	pentadienoic	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:10
L21	93	l1 near20 l20	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:06
L22	35	"112429"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:06
L23	197168	("514").CLAS.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 08:10
L24	164	I20 and I23	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 08:29

# **EAST Search History**

L25	2	("5675033").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 08:13
L26	14	"6238649"	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	ON	2007/12/11 10:11
L27	2	("5010189").PN.	US-PGPUB; USPAT; EPO; JPO; DERWENT	OR	OFF	2007/12/11 10:11

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         JUL 02
NEWS
         JUL 02
NEWS
                 SCISEARCH enhanced with complete author names
NEWS
         JUL 02
                 CHEMCATS accession numbers revised
NEWS
      5
         JUL 02
                 CA/CAplus enhanced with utility model patents from China
NEWS
         JUL 16
                 CAplus enhanced with French and German abstracts
NEWS
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         JUL 18
                 CA/CAplus patent coverage enhanced
         JUL 26
NEWS
      Я
                 USPATFULL/USPAT2 enhanced with IPC reclassification
      9
         JUL 30
NEWS
                 USGENE now available on STN
                 CAS REGISTRY enhanced with new experimental property tags
NEWS 10
         AUG 06
NEWS 11
         AUG 06
                 FSTA enhanced with new thesaurus edition
                 CA/CAplus enhanced with additional kind codes for granted
NEWS 12
         AUG 13
                 patents
NEWS 13
         AUG 20
                 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 14
         AUG 27
                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
NEWS 15
         AUG 27
                 USPATOLD now available on STN
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                 CAS REGISTRY enhanced with additional experimental
         AUG 28
                 spectral property data
NEWS 17
         SEP 07
                 STN AnaVist, Version 2.0, now available with Derwent
                 World Patents Index
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         SEP 13
                 FORIS renamed to SOFIS
NEWS 19
         SEP 13
                 INPADOCDB enhanced with monthly SDI frequency
NEWS 20
         SEP 17
                 CA/CAplus enhanced with printed CA page images from
                 1967-1998
         SEP 17
NEWS 21
                 CAplus coverage extended to include traditional medicine
                 patents
NEWS 22
         SEP 24
                 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 23
         OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt |
         OCT 19
NEWS 24
                 BEILSTEIN updated with new compounds
NEWS 25
         NOV 15
                 Derwent Indian patent publication number format enhanced
NEWS 26
         NOV 19
                 WPIX enhanced with XML display format
NEWS 27
         NOV 30
                 ICSD reloaded with enhancements
                 LINPADOCDB now available on STN
NEWS 28
         DEC 04
NEWS EXPRESS
             19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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=> file reg
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http://www.cas.org/support/stngen/stndoc/properties.html

#### => 2,4-pentadieneoic acid/cn

L1 0 2,4-PENTADIENEOIC ACID/CN

		_				
=>	e	2.	4-pen	itadi er	eoic.	acid/cn

E12

-> C 2,4 pcm	-aarcii	COTC acta, ch
E1	1	2,4-PENTADIENENITRILE-5-D, 5-(6,6-DIMETHYL-1-CYCLOHEXEN-1-YL
		-2-D)-3-METHYL-, (E,E)-/CN
E2	1	2,4-PENTADIENENITRILE-5-D, 5-(6,6-DIMETHYL-1-CYCLOHEXEN-1-YL
		-2-D) $-3-METHYL-$ , $(Z,E)-/CN$
E3	0>	2,4-PENTADIENEOIC ACID/CN
E4	1	2,4-PENTADIENEPEROXOIC ACID, 5-PHENYL-, 1,1-DIMETHYLETHYL ES
		TER/CN
E5	1	2,4-PENTADIENESELENOAMIDE, 2-(1,1-DIMETHYLETHYL)-N,N-DIETHYL
		-/CN
E6	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-2-(TRIMETHYLSILYL)-/C
		N
E7	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-3-METHYL-2-(TRIMETHYL
		SILYL)-, (E)-/CN
E8	1	2,4-PENTADIENESELENOAMIDE, N,N-DIETHYL-3-METHYL-2-(TRIMETHYL
		SILYL)-, $(Z)$ -/CN
E9	1	2,4-PENTADIENETHIAL/CN
E10	1	2,4-PENTADIENETHIAL, (Z)-/CN
E11	1	2,4-PENTADIENETHIAL, 2-METHYL-/CN

2,4-PENTADIENETHIAL, 3-HYDROXY-/CN

```
=> e 2,4-pentadienoic acid/cn
                      2,4-PENTADIENOHYDROXAMIC ACID, 4-METHYL-5-(5-NITRO-2-FURYL)-
E1
                      /CN
E2
               1
                      2,4-PENTADIENOHYDROXAMIC ACID, N,5-DIPHENYL-/CN
E3
               1 --> 2,4-PENTADIENOIC ACID/CN
E4
                      2,4-PENTADIENOIC ACID AMIDE/CN
                      2,4-PENTADIENOIC ACID N-METHYLAMIDE/CN
E5
               1
               1
                      2,4-PENTADIENOIC ACID, (1R,2S)-2-PHENYLCYCLOHEXYL ESTER, (2E
E6
                      )-REL-/CN
                      2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYL-1-PHE
               1
E7
                      NYLETHYL) CYCLOHEXYL ESTER, (2E) -REL-/CN
                      2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYLETHYL)
E8
               1
                      CYCLOHEXYL ESTER, (2E)-/CN
                      2,4-PENTADIENOIC ACID, (2E)-/CN
E9
               1
E10
               1
                      2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA
                      NAMINE (1:1)/CN
                      2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA
E11
               1
                      NAMINE (1:1), HOMOPOLYMER/CN
E12
                      2,4-PENTADIENOIC ACID, (2E)-2,4-PENTADIENYL ESTER, (2E)-/CN
               1
=> e 2,4-pentadienoic acid, 5-methyl/cn
                      2,4-PENTADIENOIC ACID, 5-METHOXY-3-(PHENYLTHIO)-5-((TRIMETHY
                      LSILYL)OXY) -, METHYL ESTER/CN
E2
                      2,4-PENTADIENOIC ACID, 5-METHOXY-3-METHYL-, METHYL ESTER/CN
               0 --> 2,4-PENTADIENOIC ACID, 5-METHYL/CN
E3
                      2,4-PENTADIENOIC ACID, 5-METHYL-2-(1-METHYL-1-PHENYLETHYL)CY
F.4
                      CLOHEXYL ESTER, (1R-(1A, 2B, 5A))-/CN
                      2,4-PENTADIENOIC ACID, 5-METHYL-2-(1-METHYLETHYL) CYCLOHEXYL
E5
               1
                      ESTER, (1R-(1A, 2B, 5A))-/CN
                      2,4-PENTADIENOIC ACID, 5-NITRO-/CN
               1
E6
                      2,4-PENTADIENOIC ACID, 5-NITRO-/CN

2,4-PENTADIENOIC ACID, 5-NITRO-, (2E,4E)-/CN

2,4-PENTADIENOIC ACID, 5-NITRO-, ETHYL ESTER/CN

2,4-PENTADIENOIC ACID, 5-NITRO-, ETHYL ESTER, (E,E)-/CN

2,4-PENTADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN

2,4-PENTADIENOIC ACID, 5-NITRO-, METHYL ESTER, (E,E)-/CN
E7
               1
E8
               1
E9
               1
               1
E10
E11
               1
E12
                      2,4-PENTADIENOIC ACID, 5-OXIRANYL-, METHYL ESTER, (E,E)-/CN
=> logoff hold
COST IN U.S. DOLLARS
                                                                             TOTAL
                                                          SINCE FILE
                                                                ENTRY
                                                                           SESSION
                                                                 7.20
                                                                              7.41
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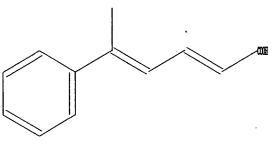
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12

chain nodes : 2 3 4 5 6 12 ring nodes : 1 7 8 9 10 11 chain bonds : 1-2 2-3 2-12 3-4 4-5 5-6 ring bonds: 1-7 1-11 7-8 8-9

9-10 10-11 exact bonds :

1-2 2-3 2-12 3-4 4-5 5-6

normalized bonds :

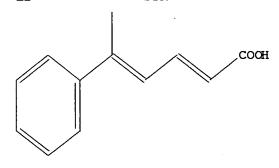
1-7 1-11 7-8 8-9 9-10 10-11

Match level:

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS

L2 STRUCTURE UPLOADED

=> d 12L2 HAS NO ANSWERS L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 12 exact sam SAMPLE SEARCH INITIATED 06:16:19 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -9 TO ITERATE

100.0% PROCESSED

9 ITERATIONS

0 ANSWERS

**SEARCH TIME: 00.00.01** 

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\*

360 PROJECTED ITERATIONS: 9 TO

PROJECTED ANSWERS: 0 TO

0 SEA EXA SAM L2 L3

=> search 12 exact full FULL SEARCH INITIATED 06:16:26 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -115 TO ITERATE

100.0% PROCESSED 115 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

3 SEA EXA FUL L2

=> d scan

REGISTRY COPYRIGHT 2007 ACS on STN L4 3 ANSWERS 2,4-Hexadienoic acid, 5-phenyl-, (Z,E)- (9CI) MF C12 H12 O2

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN L4

Sorbic acid, 5-phenyl- (6CI) IN

MF C12 H12 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

REGISTRY COPYRIGHT 2007 ACS on STN 3 ANSWERS L42,4-Hexadienoic acid, 5-phenyl-, (E,E)- (9CI) IN C12 H12 O2 MF

Double bond geometry as shown.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

#### ALL ANSWERS HAVE BEEN SCANNED

=> file caplus
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FULL ESTIMATED COST

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=> 14

L5 9 L4

=> d 15 1-9 ti

- L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Structure-antitranspirant activity relation in a series of abscisic acid analogs
- L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Influence of the substituent and the geometry of the double bond on dissociation constants of cinnamylideneacetic acids
- L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Several dichlorobutadienyl alcohols and their transformation into dienic acids
- L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis of polyene acids and aldehydes derived from dichloroacrolein
- L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Ketones with a cyclopropane nucleus. II. Some 2-oxobenzobicyclo[0.1.4]hept-3-ene compounds substituted in position 5
- L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Ketones with a cyclopropane nucleus. I. Benzo- and

### naphthobicyclo[0.1.4]heptenones

- ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN L5
- Hydroxytriazenes of anthraquinone ΤI
- T.5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
- ΤI Stereochemistry of the 1-methyl-2-carboxy-1,2,3,4-tetrahydronaphthalenes and the 5-methylbenzobicyclo[0.1.4]-hept-3-en-2-ones
- ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN L5
- Reformatskii reactions with methyl  $\gamma$ -bromocrotonate TТ

=> file req

COST IN U.S. DOLLARS

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FULL ESTIMATED COST

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=> file caplus COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.45 78.53

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(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

FILE 'REGISTRY' ENTERED AT 06:08:12 ON 11 DEC 2007

L1 0 2,4-PENTADIENEOIC ACID/CN

E 2,4-PENTADIENEOIC ACID/CN E 2,4-PENTADIENOIC ACID/CN

E 2,4-PENTADIENOIC ACID, 5-METHYL/CN

L2 STRUCTURE UPLOADED

L3 0 SEARCH L2 EXACT SAM

L4 3 SEARCH L2 EXACT FULL

FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007

L5 9 L4

FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

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=> e 2,4-pentadienoic acid/cn

E1 2,4-PENTADIENOHYDROXAMIC ACID, 4-METHYL-5-(5-NITRO-2-FURYL)-

/CN

E2 2,4-PENTADIENOHYDROXAMIC ACID, N,5-DIPHENYL-/CN

```
1 --> 2,4-PENTADIENOIC ACID/CN
E3
E4
             1
                   2,4-PENTADIENOIC ACID AMIDE/CN
F.5
             1
                   2,4-PENTADIENOIC ACID N-METHYLAMIDE/CN
                   2,4-PENTADIENOIC ACID, (1R,2S)-2-PHENYLCYCLOHEXYL ESTER, (2E
E6
             1
                   )-REL-/CN
                   2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYL-1-PHE
             1
E7
                   NYLETHYL) CYCLOHEXYL ESTER, (2E)-REL-/CN
                   2,4-PENTADIENOIC ACID, (1R,2S,5R)-5-METHYL-2-(1-METHYLETHYL)
E8
             1
                   CYCLOHEXYL ESTER, (2E) -/CN
                   2,4-PENTADIENOIC ACID, (2E)-/CN
E9
                   2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA
E10
                   NAMINE (1:1)/CN
                   2,4-PENTADIENOIC ACID, (2E)-, COMPD. WITH 1-NAPHTHALENEMETHA
E11
             1
                   NAMINE (1:1), HOMOPOLYMER/CN
E12
             1
                   2,4-PENTADIENOIC ACID, (2E)-2,4-PENTADIENYL ESTER, (2E)-/CN
=> e3
L6
             1 "2,4-PENTADIENOIC ACID"/CN
=> d 16
L6
    ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN
    626-99-3 REGISTRY
ED
    Entered STN: 16 Nov 1984
     2,4-Pentadienoic acid (CA INDEX NAME)
OTHER CA INDEX NAMES:
    \alpha, \gamma-Pentadienoic acid (3CI)
OTHER NAMES:
    β-Vinylacrylic acid
    1,3-Butadiene-1-carboxylic acid
CN
    1-Carboxy-1,3-butadiene
CN
    1-Carboxybutadiene
CN
    Butadiene-1-carboxylic acid
CN
    NSC 16628
    C5 H6 O2
MF
     COM
CI
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LC
       CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, IFICDB, IFIPAT, IFIUDB,
       SPECINFO, TOXCENTER, USPAT2, USPATFULL, USPATOLD
         (*File contains numerically searchable property data)
     Other Sources: EINECS**
         (**Enter CHEMLIST File for up-to-date regulatory information)
H2C == CH - CH == CH - CO2H
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
             155 REFERENCES IN FILE CA (1907 TO DATE)
              14 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             156 REFERENCES IN FILE CAPLUS (1907 TO DATE)
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COST IN U.S. DOLLARS
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7.35

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FILE 'CAPLUS' ENTERED AT 06:29:37 ON 11 DEC 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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960327 THU/RL

L7 2 L6/THU

(L6 (L) THU/RL)

=> d 17 1-2 ti fbib abs

- L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Use of pentadienoic acid derivatives for the treatment of hyperuricemia
- AN 2005:523273 CAPLUS
- DN 143:53517
- TI Use of pentadienoic acid derivatives for the treatment of hyperuricemia
- IN Boizel, Robert; Fouqueray, Pascale; Guerrier, Daniel; Zeiller, Jean-Jacques; Brutzkus, Bertrand
- PA Merck Patent G.m.b.H., Germany
- SO PCT Int. Appl., 64 pp. CODEN: PIXXD2

DT Patent

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$$(R)_p$$
 $R^1$ 
 $R^2$ 
 $R^2$ 

The use of a pentadienoic acid derivative of formula I (e.g., (2E, 4E)-5-(3,3-dimethyl-7-methoxy-2,3-dihydrobenzoxepin-5-yl)-3-methylpenta -2,4-dienoic acid ) is claimed for the preparation of a medicament for the prevention or treatment of hyperuricemia and/or one or several associated disorders or diseases, and/or for reducing the serum uric acid level of a subject. Medical compns. for these prevention and/or treatment, comprising such a pentadienoic acid derivative

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

#### ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
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  AN 2005:467780 CAPLUS
  DN 143:1300
  TI Use of pentadienoic acid derivatives for the prevention and/or the treatment of hyperuricemia
  IN Boizel, Robert; Fouqueray, Pascale; Guerrier, Daniel; Zeller,
- Jean-Jacques; Brutzkus, Bertrand
- PA Merck Sante, Fr. SO Eur. Pat. Appl., 45 pp.
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				US	2003-527773P	P	20031209
				WO	2004-EP12381	W	20041102
US	2007099854	A1	20070503	US	2006-580602		20060525
				EP	2003-292973	Α	20031128
				US	2003-527773P	P	20031209
				WO	2004-EP12381	W	20041102

OS MARPAT 143:1300

AB Use of pentadienoic acid derivs. for the prevention and/or the treatment of hyperuricemia and/or associated disorders or diseases. The use of a pentadienoic acid derivative of formula (I) for the preparation of a medicament for

the prevention or treatment of hyperuricemia and/or one or several associated disorders or diseases, and/or for reducing the serum uric acid level of a subject. Medical compns. for these prevention and/or treatment, comprising such a pentadienoic acid derivative

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
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http://www.cas.org/support/stngen/stndoc/properties.html

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> ENTRY SESSION

SINCE FILE

FULL ESTIMATED COST

0.45 110.25

TOTAL

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

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FILE COVERS 1907 - 11 Dec 2007 VOL 147 ISS 25 FILE LAST UPDATED: 10 Dec 2007 (20071210/ED)

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=> 16/prep

156 L6

4500485 PREP/RL

L8

33 L6/PREP

(L6 (L) PREP/RL)

=> d 18 30-33 ti

- ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid TΙ
- ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- 2,4-Pentadienoic acids
- L8 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- ΤI Butadienyl compounds
- 1.8 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- ΤI A hypothesis on the biological origin of resin acids
- => d 18 28-33 ti fbib abs
- ANSWER 28 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- ΤI Acetylenic compounds. XLV. The alkaline isomerization of but-3-ynoic acid
- AN 1955:60249 CAPLUS
- DN 49:60249
- OREF 49:11555i,11556a-d
- TI Acetylenic compounds. XLV. The alkaline isomerization of but-3-ynoic acid
- AU Eglinton, G.; Jones, E. R. H.; Mansfield, G. H.; Whiting, M. C.

CS Univ. Manchester, UK

SO Journal of the Chemical Society (1954) 3197-3200 CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

OS CASREACT 49:60249

AB cf. C.A. 49, 8142f. A study has been made of the effect of alkali on but-3-ynoic acid (I). Under the mild conditions of heating 3 hrs. at 40° with 18% K2CO3 solution, a 92% yield of buta-2,3-dienoic acid (II), m. 65-6° (from light petroleum) was obtained. More vigorous treatment (18% K2CO3 at 90° for 6 hrs.) gave further isomerization to but-2-ynoic acid (III), m. 75-6° (from light petroleum). Et but-3-ynoate (IV), b. 104-5°/190 mm., n19D 1.4291, isomerized much more readily than the acid. Even KHCO3 solution at 50° gave Et buta-2,3-dienoate (V), b. 44°/130 mm., n19D 1.4585, and with 10% K2C03 at  $20^{\circ}$ , the reaction went almost to completion. V was found to be extremely reactive toward nucleophilic reagents. Treating V with an EtOH solution of NaOEt gave Et  $\beta$ -ethoxycrotonate (VI). Piperidine also added to V to form Et  $\beta$ -piperidinocrotonate, b. 110° (bath temperature)/0.03 mm., n16D 1.5392,  $\lambda$ maximum 2870 A.,  $\epsilon$  = 24700. V and aniline yielded Et  $\beta$ -anilinocrotonate, b.  $106^{\circ}/0.5$  mm., n16D 1.5820,  $\lambda maximum 3010 A., <math>\epsilon = 20400$ , and with p-phenetidine and V, there resulted Et  $\beta$ -p-ethoxyanilinocrotonate, m. 53-4°,  $\lambda$ maximum 2960 A.,  $\epsilon$  = 22800. When a solution of II in xylene was refluxed, there was gradual polymerization and a little dehydroacetic acid was isolated. Partial hydrogenation of II in EtOAc in the presence of 1.5% Pd on CaCO3 gave cis-crotonic acid, which, on bromination, gave a 70% yield of threo- $\alpha, \beta$ -dibromobutyric acid, m. 58-9° (from pentane). Reaction of II and V with LiAlH4 was also studied. II gave primarily vinylacetic acid, b. 85° (bath temperature)/16 mm., n23D 1.4218, and some but-3-en-1-ol, b. 112°/767 mm., n21D 1.4180;  $\alpha$ -naphthylurethan, m. 76-7°. A similar reduction of V gave Et vinylacetate, b. 75°/130 mm., n21D 1.4110, and a small quantity of but-3-en-1-ol.

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L8 ANSWER 29 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
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TI 2,4-Pentadienoic acids

AN 1952:42374 CAPLUS

DN 46:42374

OREF 46:7114i

TI 2,4-Pentadienoic acids

PA N. V. de Bataafsche Petroleum Maatschappij

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE .	APPLICATION NO.	DATE
	PATENT NO.	KIND	DITTED .		
PI	GB 668569		19520319	GB 1949-18473	19490713

AB See U.S. 2,515,595 (C.A. 44, 9979b).

L8 ANSWER 30 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

TI Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid

AN 1951:26931 CAPLUS

DN 45:26931

OREF 45:4683e-i,4684a-d

TI Diene syntheses. XXVI. A dimeric butadiene-1-carboxylic acid

AU Alder, Kurt; Vogt, Wilhelm

CS Univ. Cologne, Germany

SO Ann. (1950), 570, 190-200

DT Journal

LA Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C.A. 44, 1066a. Details are given for the preparation and purification of

CH2:CHCH:CHCO2H (I), b12 102-3°, m. 72°, formed from CH2(CO2H)2 and acrolein. I (31 q.) refluxed 24 hrs. with 2% each methylene blue and p-(HO)2C6H4 in 155 g. xylene, followed by extraction with hot aqueous Na2CO3, acidification, and extraction with Et2O gave about 40% of a crystalline dimer (II), m. 147° (from AcOEt), and 40% of an oily mixture (III), together with a tacky polymeric mixture II (2 g.) heated 2 hrs. with 3.3 g. Br at 200°, followed by solution in aqueous Na2CO3, filtration, and debromination with Na-Hg and treatment at 0° with 5% KMnO4, gave o-HO2CC6H4CH2CH2CO2H, m. 165-6° (cf. Straus and Lemmel, C.A. 7, 1499). II (0.5 g.) warmed 2-3 min. with 15 parts concentrated H2SO4, rapidly cooled, poured on ice, and extracted with Et20 gave a mixture of 1,2-C6H4.CO.O.CHCH2CO2H, m. 152° (cf. Roth, C.A. 8, 2724) and a new hydrindonecarboxylic acid, C10H8O3 (IV), m. 222-3° (from AcOEt) (semicarbazone, decompose 285°), whose (impure) Me ester m. 102° [semicarbazone, C12H13O3N3, needles, decompose 259° (from AcOAm)]. Catalytic hydrogenation of II with PtO2 in AcOH proceeded at a constant rate (indicating absence of appreciable amts. of an isomer) and yielded a cis-dihydro derivative (V) of II, m. 128°; Me ester, oil. Refluxed 8 hrs. with 5 cc. 40% KOH, 1 g. V gave, after acidification, trans-HO2CCH.(CH2)4.CHCH:CHCO2H (VI), m. 180°, which oxidized with cold alkaline KMnO4 gave 1,2-(HO2C)2C6H10, m. 219-20° (Diels and Alder, C.A. 22, 1144). Refluxing VI with 50 parts 10% H2SO4 yielded the trans-lactone, C10H14O4, m. 119° and depressing the m.p. of V. Refluxing II 0.5 hr. with 5 parts 40% KOH, followed by acidification and Et20 extraction, gave the compound (VII), m. 136° and depressing the m.p. of II. When hydrogenated, VII gave V, but when II was refluxed 20 hrs. with 40% KOH, it yielded a dienedicarboxylic acid, HO2CC:C(CH:CHCO2H).CH2.CH2.CH2.CH2 (VIII), m. (poorly due to lactonization) 158-63° (from AcOH), readily isomerized by hot aqueous H2SO4 to CH2.(CH2)2.CH2.C:C.CH(CH2CO2H).O.CO, m. 114-15°. The latter wag unsatd. toward KMnO4, but failed to add H at room temperature when treated with PtO2 in AcOH. Under similar conditions, VIII proved difficult to hydrogenate; even after 3 days a portion (m. 157° from Et20) remained unsatd. toward KMnO4, but was apparently not identical with VIII and remained unchanged on heating with aqueous H2SO4. The only hydrogenated portion obtained from VIII was converted through its acid chloride into 2-PhNHCOC6H10CH2CH2CONHPh, m. 212° (cf. Huckel, C.A. 19, 1269). III was a mixture of 75% mono- and 25% dibasic acids, which with concentrated H2SO4 gave IV. Catalytic hydrogenation of III gave small amts. of V and a brown oil, which when refluxed 24 hrs. with 40% KOH, diluted, and oxidize with 5% KMnO4, yielded about 10% 1,2-(HO2C)2C6H10. III with CH2N2 gave a mixture, of which the fraction b12 175-90° gave on saponification VIII and a compound m. 211° (yielding a hydrogenation product, m. 188°, not identical with VI); another fraction, b12 190-210°, when saponified gave small amts. of VIII.

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ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
rs
TI
     2.4-Pentadienoic acids
     1950:52175 CAPLUS
AN
     44:52175
DN
OREF 44:9979b-d
ΤI
     2,4-Pentadienoic acids
IN
     Geyer, Bradford P.; Ballard, Seaver A.
PA
     Shell Development Co.
DT
     Patent
```

LΑ

Unavailable

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IIS 2515595		19500718	IIS 1948-39817	19480720

PIUS 1948-39817 A 2,4-pentadienoic acid is produced by the liquid-phase condensation of an AB

 $\alpha$ -methylenealkanal with CH2:CO (I) in the presence of a basic catalyst. Thus, into CH2:CHCHO (II) 84 g. (containing 0.1% p-(HO)2C6H4 and NaOAc 10 g. in Et2O 200 cc. at  $-30^\circ$  is passed I (more than 52 g. in 4 hrs.), the mixture filtered, the filtrate distilled to remove II and Me2CO, the residue (128 g.) neutralized at  $0^\circ$  with aqueous NaOH, 300 cc. HCCl3 added, the mixture acidified with 25% HCl at  $0^\circ$ , the HCCl3 layer dried and distilled at 0.2 mm., and CH2:CHCH:CHCO2H, m. 71°, isolated by sublimation.

L8 ANSWER 32 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN

TI Butadienyl compounds

AN 1937:25080 CAPLUS

DN 31:25080

OREF 31:3503h-i,3504a-c

TI Butadienyl compounds

IN Carothers, Wallace H.; Berchet, Gerard J.

PA E. I. du Pont de Nemours & Co.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	·				
ΡI	US 2073363		19370309	US 1932-640326	19321029
AB				by heating 4-chloro-1,	
	with an oxide or ca	arbonate	such as Ca(	or Na2CO3 in water at	60-90°

with an oxide or carbonate such as CaO or Na2CO3 in water at 60-90° for 15 hrs.; by fractional distillation, a purified product is obtained which

is

a colorless liquid b756 126-8° which has a powerful vesicant action on the skin and the vapor of which has a strongly irritating effect upon the mucous membranes. It tends to polymerize when heated. By reaction with Me2SO4, etc., alkyl ethers of the hydroxy-1,2-butadiene are formed, and aromatic ethers are formed from it by reaction with metallic phenolates. Details are also given of the production of 4-phenoxy-1,2-butadiene, esters such as the formic, acetic, trichloroacetic, succinic, benzoic, phthalic and p-nitrobenzoic esters, the chlorocarbonic ester, b57  $66-8^{\circ}$  and suitable for use in the preparation of urethans having medicinal properties or the production of different esters by reaction with an alc. or a phenol, and of the production of butadienyl thiocyanate, butadienyl chloride, butadienyl cyanide,  $\beta$ ,  $\delta$ -dimethoxyvaleronitrile, polymerized butadienyl cyanide, ethyl  $\beta$ -vinyl acrylate (which polymerizes to a rubber-like mass on heating to 100° for 10 hrs.), β-vinylacrylic acid and a polymer, various amines of 4-hydroxy-1,2-butadiene,  $\alpha$ -N-naphthyl-N'-2,3-butadienyl-1-urea, m. 77°, di- and tri-(2,3butadienyl)amines, mono(2,3-butadienyl)aniline, di(2,3-butadineyl)aniline, butadienylacetic acid, butadienylacetone, ethylbutadienylbarbituric acid, isomers and dehydration products of 4-hydroxy-1,2-butadiene, methyl, ethyl, butyl, heptyl, butadienyl and phenylethyl esters of butadienylacetic and of methylethenylpropionic acids, butadienyl mercaptan and butadienyl sulfide, phenyl-p-tolylbutadienylcarbinol, etc. The butadienylamines may be used for the manufacture of dyes and pharmaceutical chemicals and for inhibiting oxidation of substances such as rubber and natural unsatd. fatty oils. Numerous details of procedure and properties of the products obtained are given.

- L8 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN
- TI A hypothesis on the biological origin of resin acids
- AN 1925:26895 CAPLUS
- DN 19:26895
- OREF 19:3485f-h
- TI A hypothesis on the biological origin of resin acids
- AU Aschan, Ossian
- SO Chemiker-Zeitung (1925), 49, 689-91 CODEN: CMKZAT; ISSN: 0009-2894
- DT Journal

#### Unavailable LΑ

cf. C. A. 15, 3096; 17, 1228; 18, 2151. The formulas of terpenes, AB polyterpenes and resin acids are all multiples of isoprene, C5H8. Their formation from this common building stone by the action of enzymes appears more probable than the formation of resin acids by oxidation of terpenes. The rubber production by tropical plants and the presence of isoprene, isoamylene and isopentane in masut suggest that isoprene is a widely spread plant metabolite in all latitudes as well as in the prehistoric epoch. The following is the hypothetical formation of isoprene (I) and vinylacrylic acid (II) from the normal intermediates of enzymic carbohydrate decomposition: Acetone, dihydroxyacetone and pyruvic acid condense with AcH to aldols, which after their reduction to the glycols split off water. The condensation of 2-4 mols. I leads to all the mono- and diterpenes of the Pinus species (abietin, pinabietin, colophene). condensation of 3 mols. I with 1 mol. II yields a hypothetical abietic acid, the structure of which resembles closely that of Virtannen's pinabietic acids.

#### => d his

L2

(FILE 'HOME' ENTERED AT 06:07:53 ON 11 DEC 2007)

FILE 'REGISTRY' ENTERED AT 06:08:12 ON 11 DEC 2007

L1 0 2,4-PENTADIENEOIC ACID/CN

> E 2,4-PENTADIENEOIC ACID/CN E 2,4-PENTADIENOIC ACID/CN

E 2,4-PENTADIENOIC ACID, 5-METHYL/CN

STRUCTURE UPLOADED

L3 O SEARCH L2 EXACT SAM

L43 SEARCH L2 EXACT FULL

FILE 'CAPLUS' ENTERED AT 06:16:55 ON 11 DEC 2007 9 L4 L5

FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

FILE 'REGISTRY' ENTERED AT 06:29:04 ON 11 DEC 2007 E 2,4-PENTADIENOIC ACID/CN

L6 1 E3

FILE 'CAPLUS' ENTERED AT 06:29:37 ON 11 DEC 2007 L7 2 L6/THU

FILE 'REGISTRY' ENTERED AT 06:32:17 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:32:27 ON 11 DEC 2007 L833 L6/PREP

=> file req

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```
=> e 5-phenyl- 2,4-pentadienoic acid/cn
             1
                   5-PHENYL MELDRUM'S ACID/CN
E2
                   5-PHENYL(1,3,4)OXADIAZOLE-2-CARBONYL CHLORIDE/CN
             0 --> 5-PHENYL- 2,4-PENTADIENOIC ACID/CN
E3
                   5-PHENYL-(1,3,4)OXADIAZOLE-2-CARBOXYLIC ACID (4-FLUORO-3-(PY
E4
             1
                   RAZIN-2-YLOXYMETHYL) PHENYL) AMIDE/CN
             1
                   5-PHENYL-(1,3,4)OXADIAZOLE-2-CARBOXYLIC ACID N-(5-((BENZOYL)
E5
                   (METHYL) AMINO) -1-(2-CARBAMOYLETHYL) -1H-BENZIMIDAZOL-2-YL) AMI
                   DE/CN
             1
                   5-PHENYL-(2E, 4E)-PENTADIENOYL CHLORIDE/CN
E6
E7
             1
                   5-PHENYL-(3S)-HYDROXY-1-PENTYNE/CN
E8
             1
                   5-PHENYL-1, 10-PHENANTHROLINE/CN
             1
                   5-PHENYL-1,2,3,4-TETRAZOLE/CN
E9
E10
             1
                   5-PHENYL-1,2,3,4-THIATRIAZOLE/CN
E11
             1
                   5-PHENYL-1,2,3,4-THIATRIAZOLE-3-OXIDE/CN
                   5-PHENYL-1,2,3-THIADIAZOLE/CN
E12
=> e 2,4-pentadienoic acid, 5-phenyl/cn
                   2,4-PENTADIENOIC ACID, 5-PHENOXY-, ETHYL ESTER/CN
F.1
             1
E2
             1
                   2,4-PENTADIENOIC ACID, 5-PHENOXY-, METHYL ESTER/CN
             0 --> 2,4-PENTADIENOIC ACID, 5-PHENYL/CN
E3
                   2,4-PENTADIENOIC ACID, 5-PHENYL-/CN
E4
             2
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENY
E5
             1
                   L)OXY)METHYL ESTER/CN
             1
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, ((2-METHYL-1-OXO-2-PROPENY
E6
                   L)OXY)METHYL ESTER, POLYMER WITH BUTYL 2-METHYL-2-PROPENOATE
                    AND 2-METHYL-2-PROPENOIC ACID/CN
E7
             1
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,2'-BIPYRIDINE)-4,4'-DIY
                   LBIS (METHYLENE) ESTER, (2E, 2'E, 4E, 4'E) -/CN
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4,6-TRIOXO-1,3,5-TRIAZI.
E8
             1
                   NE-1,3,5(2H,4H,6H)-TRIYL)TRI-2,1-ETHANEDIYL ESTER/CN
             1
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, (2,4-DICHLOROPHENYL) (DIETH
E9
                   OXYPHOSPHINYL) METHYL ESTER, (2E, 4E) -/CN
E10
             1
                   2,4-PENTADIENOIC ACID; 5-PHENYL-, (2-CHLOROPHENYL) (DIETHOXYP
                   HOSPHINYL) METHYL ESTER, (2E, 4E) -/CN
E11
             1
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, (2E)-4-ETHOXY-4-OXO-2-BUTE
                   N-1-YL ESTER, (2E, 4E)-/CN
E12
             1
                   2,4-PENTADIENOIC ACID, 5-PHENYL-, (2E,4E)-/CN
=> e4
L9
             2 "2,4-PENTADIENOIC ACID, 5-PHENYL-"/CN
```

L9 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2007 ACS on STN

RN 54352-97-5 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,4-Pentadienoic acid, 5-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Juarezic acid

MF C11 H10 O2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CHEMINFORMRX, IFICDB, IFIUDB (\*File contains numerically searchable property data)

Ph-CH=CH-CH=CH-CO2H

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> 19

L10 158 L9

=> 9/thu

0 9/CT 960327 THU/RL L11 0 9/THU

(9/CT (L) THU/RL)

=> 19/thu

158 L9

960327 THU/RL

L12 10 L9/THU

(L9 (L) THU/RL)

- => d l12 1-10 ti
- L12 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Prosthetic implant materials containing donepezil, and artificial tissue containing the same
- L12 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Method for manufacturing tissue body with implant materials containing donepezil, and implant materials
- L12 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Visible light-curable materials and their use for wound healing promoters
- L12 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Physiologically active substance-coated stents, their manufacture, and sustained-release drug delivery using them
- L12 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Energy properties of statistical copolymer thin films as a measure of their biocompatibility with oncological medicine
- L12 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells
- L12 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Induction of histone acetylation and inhibition of growth by phenyl alkanoic acids and structurally related molecules
- L12 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- L12 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- L12 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Structure-antibacterial activity relationship of some aromatic acids
- => d 112 6-10 ti fbib abs
- L12 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells
- AN 2004:733540 CAPLUS
- DN 141:325331
- TI The novel histone deacetylase inhibitor BL1521 inhibits proliferation and induces apoptosis in neuroblastoma cells
- AU de Ruijter, Annemieke J. M.; Kemp, Stephan; Kramer, Gertjan; Meinsma, Rutger J.; Kaufmann, Judith O.; Caron, Huib N.; van Kuilenburg, Andre B.

Ρ.

- CS Laboratory Genetic Metabolic Diseases, Department of Paediatrics/Emma Children's Hospital and Clinical Chemistry, Academic Medical Centre, University of Amsterdam, Amsterdam, 1100 DE, Neth.
- SO Biochemical Pharmacology (2004), 68(7), 1279-1288 CODEN: BCPCA6; ISSN: 0006-2952
- PB Elsevier B.V.
- DT Journal
- LA English
- Neuroblastoma is a childhood cancer arising from the sympathetic nervous AB system. Disseminated neuroblastoma has a poor prognosis despite intensive multimodality treatment. Histone deacetylases (HDACs) were recently discovered as a potential target for pharmacol. gene therapy in cancer. HDACs have an important function in regulating DNA packaging in chromatin, thereby affecting the transcription of genes. In this paper, we tested the efficacy of a newly developed histone deacetylase inhibitor, BL1521, on neuroblastoma in vitro by investigating the changes in: acetylation of histone H3, in situ HDAC activity, p21WAF1/CIP1 and MYCN expression, metabolic activity, proliferation, morphol. and the amount of apoptosis present. BL1521 inhibited the in situ HDAC activity of a panel of neuroblastoma cell lines by at least 85%. Western anal. showed an increase of histone H3 acetylation in neuroblastoma cells after incubation with BL1521. Northern anal. showed an increase in the expression of p21WAF1/CIP1 and a decrease in the expression of MYCN in neuroblastoma cells after incubation with BL1521. Proliferation as well as the metabolic activity of neuroblastoma cells decreased significantly in response to treatment with BL1521, regardless of the MYCN status of the cells. BL1521 induced poly-(ADP-ribose) polymerase cleavage in a timeand dose-dependent manner, indicating the induction of apoptosis. Furthermore, when compared to the HDAC inhibitors Trichostatin A and 4-phenylbutyrate, BL1521 has an intermediate efficacy. Our results show that BL1521 is a potent inhibitor of HDAC and that HDACs are an attractive target for selective chemotherapy in neuroblastoma.
- RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L12 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Induction of histone acetylation and inhibition of growth by phenyl alkanoic acids and structurally related molecules
- AN 2004:450167 CAPLUS
- DN 142:32394
- TI Induction of histone acetylation and inhibition of growth by phenyl alkanoic acids and structurally related molecules
- AU Lea, Michael A.; Shareef, Asif; Sura, Monali; desBordes, Charles
- CS Department of Biochemistry and Molecular Biology, UMDNJ-New Jersey Medical School, Newark, NJ, 07103, USA
- SO Cancer Chemotherapy and Pharmacology (2004), 54(1), 57-63 CODEN: CCPHDZ; ISSN: 0344-5704
- PB Springer-Verlag
- DT Journal
- LA English
- AB Purpose. A structure-activity study was undertaken to determine the influence of side chain length of Ph alkanoic acids and the degree of unsath. of Ph alkenoic acids on the induction of histone acetylation and inhibition of cancer cell proliferation. Materials and methods. Studies on cell proliferation were performed with DS19 mouse erythroleukemic cells, PC-3 human prostate cancer cells and Caco-2 human colon cancer cells. Actions on histone deacetylase and the induction of histone acetylation were compared for 4-phenylbutyrate and structurally related mols. Results. Increasing inhibition of cell proliferation by Ph alkanoic acids together with a decrease in cells in S phase and an increase in apoptotic cells was observed with increased chain length between four and ten carbons. Introduction of double bonds into the side chain was associated with

increased growth inhibition. In contrast, 4-phenylbutyrate was a more potent inhibitor of histone deacetylase and inducer of histone acetylation than the other Ph alkanoic acids examined Conclusions. In comparison with the action of 4-phenylbutyrate, actions other than inhibition of histone deacetylase appear to be more important for growth inhibition by longer chain Ph alkanoic and Ph alkenoic acids.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L12 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- AN 2002:755220 CAPLUS
- DN 137:262850
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- IN Lan-Hargest, Hsuan-yin; Kaufman, Robert J.; Wiech, Norbert L.
- PA USA
- SO U.S. Pat. Appl. Publ., 19 pp.
  - CODEN: USXXCO
- DT Patent
- LA English
- FAN.CNT 8

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AB Title compds. AY1LY2C(:X1)X2 (I) [wherein A = (un)substituted (hetero)cycloalkyl, (hetero)cycloalkenyl, (hetero)aryl; or A =

(un) substituted hydrocarbon chain interrupted by O, S, NRa, CO, NRaSO2, SO2NRa, NRaCO2, OCONRa, NRaCONRb, OCO, CO2, OSO2, SO2O, or OCO2; Y1 and Y2 = independently CH2, O, S, NRc, NRcCO2, OCONRc, NRcCONRd, OCO2, or a bond; Ra, Rb, Rc, and Rd = independently H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, or haloalkyl; L = (un)substituted straight hydrocarbon chain optionally containing at least one double and/or triple bond; X1 = O or S; X2 = OR1, SR1, NR3OR1, NR3SR1, CO2R1, CHR4OR1, N:NCON(R3)2, or OCHR4OCOR5; R1 and R2 = independently H, (hydroxy)alkyl, haloalkyl, or hydroxy protecting group; R3 = H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, haloalkyl, or amino protecting group; R4 = OH, (hydroxy)alkyl, or haloalkyl; R5 = (hydroxy)alkyl or haloalkyl; provided that when L = Et or Pr and X2 = OR1, then Y1  $\neq$  a bond and Y2  $\neq$  a bond; or salts thereof] where prepared with Zn-binding moieties, such as hydroxamic acid or carboxylic acid groups, for inhibiting histone deacetylation activity in cells. For example, Et (trans)-cinnamate was treated with MeMqI in anhydrous ether to give 4-phenyl-2-methyl-3-buten-2-ol, which was converted to 3-methyl-5-phenyl-2,4-pentadienal using PO3Cl in DMF. Oxidation of the aldehyde with aqueous AgNO3 in EtOH afforded the desired 3-methyl-5-phenyl-2,4pentadienoic acid (II). Test compds. of the invention showed potent inhibition of histone deacetylase with IC50 values in the low µM range; e.g. two test compds. showed IC50 values of 1.7  $\mu M$  and 1.9  $\mu M$ . Histone deacetylase inhibition can repress gene expression, including expression of genes related to tumor suppression. Thus, I provide an alternate route for treating cancer, hematol. disorders, e.g., hemoglobinopathies, and genetic related metabolic disorders, e.g., cystic fibrosis and adrenoleukodystrophy (no data).

- L12 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- AN 2002:754352 CAPLUS
- DN 137:262849
- TI Preparation of arylalkanoic acids and hydroxamic acids as histone deacetylase inhibitors for treatment of cancer, hematological disorders, and genetic related metabolic disorders
- IN Lan-Hargest, Hsuan-Yin; Kaufman, Robert J.; Wiech, Nobert L.
- PA Circagen Pharmaceutical, USA
- SO PCT Int. Appl., 66 pp. CODEN: PIXXD2
- DT Patent
- LA English

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                                               US 2002-427567P
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				US 2002-427567P WO 2003-US36981	P W	20021120 20031119
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AB

Title compds. AY1LY2C(:X1)X2 (I) [wherein A = (un)substituted (hetero)cycloalkyl, (hetero)cycloalkenyl, (hetero)aryl; or A = (un) substituted hydrocarbon chain interrupted by O, S, NRa, CO, NRaSO2, SO2NRa, NRaCO2, OCONRa, NRaCONRb, OCO, CO2, OSO2, SO2O, or OCO2; Y1 and Y2 = independently CH2, O, S, NRc, NRcCO2, OCONRc, NRcCONRd, OCO2, or a bond; Ra, Rb, Rc, and Rd = independently H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, or haloalkyl; L = (un) substituted straight hydrocarbon chain optionally containing at least one double and/or triple bond; X1 = O or S; X2 = OR1, SR1, NR3OR1, NR3SR1, CO2R1, CHR4OR1, N:NCON(R3)2, or OCHR4OCOR5; R1 and R2 = independently H, (hydroxy)alkyl, haloalkyl, or hydroxy protecting group; R3 = H, (hydroxy)alkyl, alkenyl, alkynyl, alkoxy, OH, haloalkyl, or amino protecting group; R4 = OH, (hydroxy)alkyl, or haloalkyl; R5 = (hydroxy) alkyl or haloalkyl; provided that when L = Et or Pr and X2 = OR1, then  $Y1 \neq a$  bond and  $Y2 \neq a$  bond; or salts thereof] where prepared with Zn-binding moieties, such as hydroxamic acid or carboxylic acid groups, for inhibiting histone deacetylation activity in cells. For example, Et (trans)-cinnamate was treated with MeMgI in anhydrous ether to qive 4-phenyl-2-methyl-3-buten-2-ol, which was converted to 3-methyl-5-phenyl-2,4-pentadienal using PO3Cl in DMF. Oxidation of the aldehyde with aqueous AgNO3 in EtOH afforded the desired 3-methyl-5-phenyl-2,4pentadienoic acid (II). Test compds. of the invention showed potent inhibition of histone deacetylase with IC50 values in the low µM range; e.g. two test compds. showed IC50 values of 1.7  $\mu$ M and 1.9  $\mu$ M. Histone deacetylase inhibition can repress gene expression, including expression of genes related to tumor suppression. Thus, I provide an alternate route for treating cancer, hematol. disorders, e.g., hemoglobinopathies, and genetic related metabolic disorders, e.g., cystic fibrosis and adrenoleukodystrophy (no data).

- L12 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Structure-antibacterial activity relationship of some aromatic acids
- AN 1998:797015 CAPLUS
- DN 130:194161
- TI Structure-antibacterial activity relationship of some aromatic acids
- AU Abeytunga, D. T. U.; Peiris, T. E. M.; Wijesundera, R. L. C.
- CS Department of Chemistry, University of Colombo, Colombo, 3, Sri Lanka
- SO Journal of the National Science Council of Sri Lanka (1998), 26(2), 133-139
  - CODEN: JNSCBH; ISSN: 0300-9254
- PB Natural Resources, Energy and Science Authority of Sri Lanka
- DT Journal
- LA English
- AB Nine aromatic acids were tested for their antibacterial effect against Staphylococcus aureus. 3-Phenylpropanoic acid was identified as the most active of the acids chosen for this bioassay. In general a 3,4-methylenedioxy substituent on the Ph group reduces the activity against Staphylococcus aureus.

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49 L13 NOT L12

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- L14 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters
- L14 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains
- L14 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type
- L14 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Unsaturated organic compounds
- L14 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Condensation of aldehydes with malonic acid. XIX. Condensation of cinnamaldehyde
- L14 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis of some 5-substituted 5-hydroxy-2-pentenoic acids
- L14 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Reformatsky condensations involving vinylogs of haloacetic esters
- L14 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI o-Methoxyphenylmalonic acid and its derivatives
- L14 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI General synthesis of  $\alpha$ -unsaturated acids from malonic acid
- L14 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Polymerization of allyl cinnamalacetate
- L14 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The distillation products of  $\alpha$ -truxilic acid. Obtainment of a fourth truxillic acid
- => d 114 39,40, 41, 47-49 ti fbib abs
- L14 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters
- AN 1953:18972 CAPLUS
- DN 47:18972
- OREF 47:3271d-e
- TI The mechanism of the reaction of bromine with 2,2-diphenylpenten-4-oic acid and its esters
- AU Lindsay, Kenneth L.
- CS Univ. of Minnesota, Minneapolis
- SO (1952) 92 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 4341 From: Dissertation Abstracts 12, 814-15
- DT Dissertation
- LA Unavailable
- AB Unavailable
- L14 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains
- AN 1953:18971 CAPLUS
- DN 47:18971
- OREF 47:3270c-i,3271a-d

- TI Reduction of unsaturated acid amides to unsaturated aldehydes; a contribution to the synthesis of polyene chains
- AU Wittig, Georg; Hornberger, Paul
- CS Univ. Tubingen, Germany
- SO Ann. (1952), 577, 11-25
- DT Journal
- LA Unavailable
- OS CASREACT 47:18971
- AB Mixed at -78° and then heated 24 hrs. at 125° in a sealed tube (or autoclave), 2.7 g. LiH and 7.1 g. BF3.Et20 in absolute Et20 gave 4 g. LiBH4.Et20 (I), extremely hygroscopic, forming a solution without decomposing Heated at 33°, I lost Et2O, giving LiBH4, m. 278-9°, exploding when heated in a free flame. Similarly formed from NaH was NaBH4, insol. in Et20, soluble in iso-PrNH2. Heated under N at 175°, 11.5 g. B(OBu)3 (II) and 0.4 g. LiH, followed by Et2O addition, gave 10 g. Li[BH(OBu)3].0.5Et20 (III), rectangles, decomposing in air, yielding H with H2O or alc., soluble in tetrahydrofuran (IIIa), slightly soluble in Et2O and C6H6, practically insol. in dioxane. II heated with excess LiH gave I. Techniques for analyzing the various Li derivs. are outlined. Ph2Zn (2.2 g.) and 0.8 g. LiH warmed to 90°, treated with Et20, and "dried" over paraffin gave 2.5 g. Li[ZnHPh2].Et20, having solubilities similar to those of III. Ph2Be from Ph2Hg (cf. C.A. 45, 5556b) was freed from xylene by distillation under N, taken up in Et2O, and separated from BeHg, giving Ph2Be.2Et2O (IV), cubes, m. 28-32°, losing Et2O when heated in vacuo at 130°. IV (3.1 g.) and 0.8 g. LiH under N at 160-5°, followed by Et20 extraction, gave Li(BeHPh2). Et20, rhombs (stored under N), decomposing in air with evolution of heat and light, giving H on treatment with H2O. PhCH:CHCOCl (V) (8.4 g.) and Ph2NH in absolute Et2O gave 13.3 g. PhCH:CHCONPh2 (VI), m. 152-3°. VI (3 g.) suspended in 15 cc. dry Et20, heated 1 hr. with M I, and treated with aqueous HCl was not reduced, but gave 90% of a stereoisomeric or polymorphic modification (VII) of VI, leaflets, m. 191-2°, which, when inoculated at 130° with VI, gave the latter. However molten VI was not converted into VII by inoculation. VII was also obtained by heating VI with LiAlH4 (VIII) in IIIa or Et2O, unless a large excess VIII was used, whereupon VII was no longer formed, but 37% PhCH:CHCH2OH, b0.1 135-8° (phenylurethan, m. 89-91°), was obtained (in the Et2O extract). V (18.3 g.) and 16.7 g. carbazole (IX), stirred 0.5 hr. at 200° cooled, triturated with 100 cc. MeOH, and cooled to 0°, gave 21 g. 9-cinnamoyl derivative (X) of IX, m. 96-6.5°. With VIII, X in Et2O at 0°, followed by addition of PhNHNH2, gave a mixture of 2.55 g. PhCH: CHCH: NNHPh, m. 166-7°, and IX (subliming from the mixture at 0.1 mm. and 120°). Ph(CH:CH)2COCl in absolute Et20 and Me2NH.HCl, treated dropwise with concentrated aqueous KOH, gave 88% Ph(CH:CH)2CONMe2 (XI), m. 109-10° (from C6H6-petr. ether). XI was not reduced by I or VIII, but with VIII gave an unstable isomer of XI (cis-trans?), m. 70-2° (from cyclohexane in the dark), reconverted into XI on standing or on repeated crystallization Ph(CH:CH)2COC1 (9.6 g.) heated with 8.4 g. IX in xylene

gave 10.1 g. 9-Ph-(CH:CH)2CO derivative (XII) of IX, lemon-yellow leaflets, m. 124-5°. I heated with XII in Et2O, followed by addition of aqueous HCl, gave 62% Ph(CH:CH)2CHO (phenylhydrazone, m. 177-9°), also formed in 72.9% yield by heating XII with VIII. Ph(CH:CH)3CHO, m. 114-15° (18.4 g.), refluxed 3 hrs. with 13.5 g. CH2(CO2H)2 in 100 cc. pyridine and

(18.4 g.), refluxed 3 hrs. with 13.5 g. CH2(CO2H)2 in 100 cc. pyridine and 1 cc. piperidine, poured into an excess aqueous H2SO4, and the resulting precipitate

decarboxylated by heating 1 hr. with 100 cc. Ac20 gave 52% Ph(CH:CH)4CO2H, yellow leaflets, m. 213-14° (from AcOH, then xylene), whose acid chloride (hygroscopic crystals) with the K derivative of IX in xylene gave 68% of the 9-Ph(CH:CH)4CO derivative (XIII) of IX, yellow needles, m. 190.5-91.5° (after crystallization from AcOEt, followed by solution in HCONMe2 and precipitation with alc.). The K derivative of IX and HO2CCH2COCl gave the 9-carboxyacetyl derivative (XIV) of IX, m. 135-7° (loss of CO2) (from

Et20, precipitated with petr. ether). Ph(CH:CH)3CHO and XIV in cold pyridine, treated with a few drops each of piperidine and AcOH and heated 2 hrs. at 70-80°, gave CO2 and (after cooling to 0°) XIII. Reduction of 10 millimoles XIII in 30 cc. IIIa with 2.5 cc. molar VIII in Et20 gave after acidification and CHCl3 extraction, 1.42 g. IX and, in the extract, 1.7

Ph(CH:CH)4CHO (XV), carmine, m. 141-3° (after sublimation at 130° and 0.1 mm.); phenylhydrazone, m. 224-6° (from HCONMe2). The reduction of XIII was also carried out with other hydrides, giving the following yields (%) of XV: with I 69, III 68, Li(ZnHPh2) 45, and Li(BeHPh2), 37. XV was separated from its contaminants by the use of Girard reagent D. In all cases 74-80% IX was also isolated. XIV and Ph(CH:CH)5CHO, m. 181-3°, under the above conditions, gave the Ph(CH:CH)6CO derivative of IX, dark red needles, m. 206-7° (from HCONMe2), which was reduced with VIII to 91% IX and 60% Ph(CH:CH)6CHO, carmine, m. 210-13° (subliming at 180° and 0.01 mm.) [phenylhydrazone, m. about 250° (decomposition)]. AcoNMe2 failed to react with PhCH:CHCHO in the presence of EtoK. The 9-Ac derivative of IX treated with PhCH:CHCHO and KOEt at 0° followed by acidification in EtoH, gave 94% IX and only about 1% (impure) XII. On the other hand, PhCH:CHCHO and 9-acetyl-4-nitrocarbazole (XVI) in absolute EtoH with KOEt gave, on acidification, 74% 4-NO2 derivative of IX, m. 208-10°, 14% XVI, and, from the alc. mother liquors, after evaporation, extraction with Et2O,

extraction of the Et2O layer (XVII) with aqueous Na2CO3, and acidification, 21% Ph(CH:CH)2CO2H, m. 163-4° (from C6H6). XVII extracted with aqueous NaHSO3 yielded 62% PhCH:CHCHO. 30 references.

- L14 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type
- AN 1951:26934 CAPLUS
- DN 45:26934

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- OREF 45:4686d-i,4687a-f
- TI Diene syntheses. XXIX. Diene syntheses with unsymmetrical addends; the 1,4-disubstituted diene type
- AU Alder, Kurt; Schumacher, Marianne; Wolff, Oswald
- CS Univ. Cologne, Germany
- SO Ann. (1950), 570, 230-50
- DT Journal
- LA Unavailable
- OS CASREACT 45:26934
- The 1,4-substituted dienes used in these expts. were all of the trans, AB trans form. PhCH:CHCH:CHMe (I) (24 g.) and 18 g. CH2:CHCO2H (II) with traces of o-C6H4(OH)2 in 100 cc. PhMe refluxed 6 hrs. gave a mixture of the following 3 isomers (in the ratio of 8:1:1): 2-cis-Phenyl-5-cis $methyl\Delta 3$ -tetrahydro-cis-benzoic acid (III), m. 159° (from AcOEt) (the main product); a 3-phenyl-6-methyl-Δ4-tetrahydrobenzoic acid (IV), m. 144-6° (from MeCN); and, from the mother liquors of IV, the 2-cis-phenyl-5-cis-methyl-Δ4-tetrahydro-trans-benzoic acid (V), m. 90-1° (from AcOEt). Dehydrogenation of III with S at 230-40° gave the new 2,5-PhMeC6H3CO2H, m. 155° (from MeCN), the crude acid chloride of which, refluxed 3.5 hrs. in 100 cc. CS2 with pure AlCl3, gave 2-methyl-9-fluorenone, m. 92° (cf. Kruber, C.A. 26, 5936). Catalytic hydrogenation of III gave a cis-dihydro derivative (VI), C14H18O2, m. 135-6°. The Me ester of VI refluxed with EtONa gave the trans-isomer of VI, m. 87° (also formed by the catalytic hydrogenation of V). Dehydrogenation of IV gave the new 3,6-PhMeC6H3CO2H, m. 209-10°. Catalytic hydrogenation of IV gave the dihydro derivative, C14H18O2, m. 142-3°. MeCH:CHCH:CHCO2H (VII) (11.2 g.), 8 g. II, and a trace of o-C6H4(OH)2, heated 5 hrs. at 135°, yielded (after digestion with Me2CO) small amts. of insol. polymers and approx. equal-amts. of the mechanically separated 5-cis-methyl-Δ3-tetrahydro-

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6-cis-methyl-Δ4-tetrahydro-cis, cis-isophthalic acid (IX), m.
    174° (both from AcOEt), together with small amts. of an oil, which,
     when dehydrogenated, gave only 2,4-(HO2C)2C6H3Me. Dehydrogenation of VIII
     gave 3,4-(HO2C)2C6H3Me. Hydrogenation of VIII gave the saturated cis-dihydro
     derivative, C9H14O4, m. 173° (decomposition), which when heated 5 hrs. at
     180° with 20 parts fuming HCl gave the trans-isomer, m.
    176°, markedly depressing the m.p. of the cis form. The di-Me
    ester of VIII (properties not given), refluxed with 10% EtONa in EtOH,
     followed by acidification, gave an isomeric "C-acid" (X), C9H12O4, m.
    228° (after Et20 extraction and crystallization from AcOEt), giving a new
     trans-dihydro derivative, m. 178-9°, marked by depressing the m.p. of
    other dihydro derivs. Dehydrogenation of IX gave 2,4-(HO2C)2C6H3Me (di-Me
    ester, m. 79°). With NaOEt (as above) IX was in small part converted into the isomeric "m-D-acid" (XI), m. 276-8° (cf.
     Wagner-Jauregg and Helmert, C.A. 33, 1269.3, who give 280°).
     Hydrogenation of IX gave a dihydro derivative, m. 195-6°, which with
     fuming HCl was rearranged into the isomeric dihydro derivative of XI, m.
    202-3° (also obtained by direct hydrogenation of XI). These
     rearrangements are discussed, but not fully explained. Refluxing the acid
     chloride (XII) of VII with CH2:CHCOCl 7 hrs. in PhMe (or in a bomb tube at
     125°), followed by addition of H2O, yielded a mixture of VIII and IX
     (but no XI). Similarly, refluxing in xylene, followed by distillation and
    hydrolysis, gave a mixture of 4 acids: 60% XI (crystallizing directly from the
aqueous
    hydrolyzate) and (on concentrating the aqueous solution), VIII, X, and a small
amount of
     an (unanalyzed) acid, m. 208°, as well as an oil, which
     dehydrogenated to 2,4-(HO2C) 2C6H3Me. XII and CH2: CHCOCl heated at
     155° in a bomb tube gave results similar to those obtained in
     xylene (with somewhat improved yields). The Me ester of VII and CH2:CHCO2Me with a trace of o-C6H4(OH)2, heated 5 hrs. at
     145-50° gave a product (XIII), b13 156 60°, saponified to XI.
     Hydrogenation of XIII in AcOEt, and saponification gave dihydro derivs. of VIII
     and IX, in approx. equal amts., and small amts. of an oil, dehydrogenated
     to 3,4-(HO2C)2C6H3Me. trans,trans-PhCH:CHCH:CHCOCl (10 g.) and 10 g.
     CH2: CHCOCl kept 30 days at room temperature, then vigorously stirred with Me2CO
     and H2O, yielded (besides 5 g. PhCH:CHCH:CHCO2H, m. 164°), 4.5 g.
     4-cis-phenyl-Δ5-tetrahydro-cis, cis-isophthalic acid (XIV), m.
     222° (from aqueous AcOH). The same reactants (18 g. and 11 g., resp.)
     heated 72 hrs. at 90-100°, followed by hydrolysis, formed 80% XIV
     (with no evidence of another isomer). When, however, the reactants were
     heated in a sealed tube at 120-30°, 60% of the products was an
     isomer (XV) of XIV, m. 245° (from MeCN). Accl or Ac20 and XIV
     yielded the anhydride, C14H12O3, m. 183° (from PhMe), readily
     reconverted into XIV. Catalytic hydrogenation of XIV gave
     4-cis-phenylhexahydro-cis, cis-phthalic acid C14H1604 (XVI), m. 213°
     (from 50% AcOH); anhydride, m. 156° (from PhMe); di-Me ester, m.
     50-1° (from MeOH). XVI (2 g.) heated 6 hrs. at 180° with
     excess fuming HCl gave a mixture of 2 trans isomers, the complete structures
     of which are still in doubt, but both of which are 4-
     phenylhexahydroisophthalic acids, 1.5 g. of the isomer (XVII) m.
     210° and 0.5 g. of the isomer (XVIII) \bar{\text{m}}. 183°.
     Hydrogenation of XV with PtO2 in AcOH yielded XVIII, which on
     dehydrogenation with SeO2 in AcOH gave 3,4-(HO2C)2C6H3Ph (XIX), m.
     245° (from AcOEt and C6H6). Attempts to cause anhydride formation
     by heating XIX with AcCl gave a noncryst. glassy material reconverted by
     long heating with H2O into XIX. Dehydrogenation of XV gave XIX. SOC12 (5
     cc.) and 0.3 g. AlCl3 refluxed 2 hrs. with 0.5 g. XIX in 20 cc. CS2,
     followed by rapid stirring with ice-H2O-HCl and by Et2O extraction, formed
     2-carboxy-9-fluorenone, subliming above 270°, identified as the Me
     ester, silky needles, m. 181° (from MeOH) [cf. Fortner, Monatsh.
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cis, cis-o-phthalic acid (VIII), m. 19374°, and

25, 451(1904)].

L14 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI General synthesis of α-unsaturated acids from malonic acid

AN 1925:19147 CAPLUS

DN 19:19147

OREF 19:2475d-f

TI. General synthesis of  $\alpha$ -unsaturated acids from malonic acid

AU Dutt, I. Sikhibhushan

SO Quart. J. Chem. Soc. (1925), 1, 297-301

DT Journal

LA Unavailable

CH2(CO2H)2 easily condenses with aldehydes in the presence of C5H11N in C5H5N solution to alkylidene- and arylidenemalonic acids, which, under the influence of C5H5N, particularly on heating, lose CO2, giving  $\alpha$ -unsatd. CO2H acids in excellent yields. AcH gives 75% of crotonic acid; 10 g. glyoxylic acid gives 1.8 g. fumaric and 2.8 g. maleic acids; BzH gives 90% of cinnamic acid; p-MeC6H4CHO gives 87% p-methylcinnamic acid; furfural gives 70% furfuracrylic acid; o-O2NC6H4CHO gives 73% o-nitrocinnamic acid; the p- and m-derivs. result in 82% and 90%, resp.; piperonal gives 76% piperonylacrylic acid; p-MeOC6H4CHO gives 80% p-methoxycinnamic acid; p-Me2NC6H4CHO gives 65% p-dimethylaminocinnamic acid; m-BrC6H4CHO gives 83% of m-bromocinnamic acid; o-HOC6H4CHO gives 20% o-coumaric acid; carbethoxyvanillin gives 12% of ferulic acid; dicarbethoxyprotocatechualdehyde gives 7% caffeic acid; PhCH:CHCHO (heating the reaction mixture 2 hrs.) gives 70% of cinnamylidenemalonic acid; on longer heating 60% of the cinnamylideneacetic acid. Me2CO gives 60% of  $\beta$ ,  $\beta$ -dimethylacrylic acid; Et2CO gives 35% of  $\beta$ ,  $\beta$ -diethylacrylic acid; cyclohexanone gives not over 5% of cyclohexylideneacetic acid.

L14 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI Polymerization of allyl cinnamalacetate

AN 1923:15035 CAPLUS

DN 17:15035

OREF 17:2419e-q

TI Polymerization of allyl cinnamalacetate

AU Blicke, F. F.

SO Journal of the American Chemical Society (1923), 45, 1562-6 CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

AB Allyl cinnamalacetate (I), obtained in 45-50% yield from allyl alc., PhCH: CHCH: CHCO2H (II) and H2SO4 at 90-5°, is light yellow, highly refractive, b20 210°, is readily saponified by alc. KOH, instantly decolorizes Br in CS2 and KMnO4 in H2O; hexabromide, m. 126°, seps. from alc. in solvated crystals, m. 111-2°. Heated in small evacuated bulbs for 7 days at 210°, I gradually becomes more and more viscous and finally changes into a light yellow, almost solid mass which, dissolved in Me2CO and poured into much cold alc., gives 25% of an amorphous, amber-like polymer of 1; this in boiling Me2CO with 5 equivs. ale, KOH (calculated on the basis of the monomol. I) gives a slightly yellow amorphous polymer of II; heated with anhydrous Ba(OH)2 this acid gives a mixture of liquid compds., undoubtedly hydrocarbons, which decolorizes Br and KMn04 and therefore contains at least 1 unsatd. constituent. Com. grades of allyl alc. and chloride undergo spontaneous polymerization on long standing.

L14 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

TI The distillation products of  $\alpha$ -truxilic acid. Obtainment of a fourth truxillic acid

AN 1923:15034 CAPLUS

DN 17:15034

OREF 17:2419c-e

- TI The distillation products of  $\alpha$ -truxilic acid. Obtainment of a fourth truxillic acid
- AU Stobbe, Hans; Zschoch, Fritz
- SO Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1923), 56B, 676-8
  CODEN: BDCBAD; ISSN: 0365-9488
- DT Journal
- LA Unavailable
- Distillation of four 30-g. portions of  $\alpha$ -truxillic acid gave at AB 90-190° 1.6 g. of a colorless aqueous liquid, at 190-290° 26.6 g. of (chiefly) trans-cinnamic acid, at 290-320° 50.7 g. of a mixture of stilbene, a compound m. 192-4°, γ-truxillic anhydride (m. 189-90°) and a new  $\eta$ -truxillic anhydride (I), above  $320^{\circ}$ , with much decomposition, 3.4 g. of a yellow-red liquid containing H2O and tarry products, and 18.1 g. residue. 1, m. 287°, depresses the m. p. of truxone (m. 294°) 30°, does not give the blue KOH melt typical of truxone, mol. weight in boiling C6H6 271-8, does not decolorize KMnO4 in Na2CO3, at 0°, is only slightly Soluble in NaOH, gives with piperidine what is probably  $\eta$ -truxillpiperididic acid, m. 240°, neutral to litmus. Digested a long time with Ba(OH)2 I gives  $\eta$ -truxillic acid, m. 260° (278-80° if previously heated a long time at 150-60% markedly depresses the m. p. of the  $\alpha$ -acid. Liebermann's "distyryl" (Ber. 22, 124(1889)) is the above mixture of 4 compds. contained in the 290-320° fraction. Distillation of 50 g. trans-cinnamic acid gave: (1) Up to 280°, chief fraction, containing 30 q. cinnamic acid and 3 g. of a neutral portion separated by further fractionation into styrene and stilbene; (2) from 280° to 310°, 1 g. of a resinous mass; (3) 8 g. of carbonized residue.

#### => d 114 28-38 ti

- L14 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Ethylenes
- L14 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis and properties of  $\alpha, \beta$ -unsaturated valerolactams
- L14 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids
- L14 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis of  $\beta$ -hydroxy esters from ethyl acetate and ketones or aldehydes by means of lithium amide. Some results with other esters
- L14 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Several dichlorobutadienyl alcohols and their transformation into dienic acids
- L14 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Phosphorus organic compounds. XX. Phosphine oxides as reagents for olefin formation
- L14 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Rearrangement of 1,1-dichloro-5-hydroxy(chloro)-5-aryl-1,3-pentadienes into  $\delta$ -arylpentadienoic acids
- L14 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The hydrolysis of  $\gamma$ -cyano- $\gamma$ -phenylpimelodinitrile
- L14 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI The reaction of acetals with malonic acid and its derivatives. A

contribution to the knowledge of the Knoevenagel-Doebner reaction

- L14 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Some new derivatives of khellin and its product of demethylation
- L14 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI An attempted synthesis of 1,10-cyclopentenoheptalene. 1,8-Tetramethyleneazulene

### => d 114 30 ti fbib abs

- L14 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids
- AN 1961:7620 CAPLUS
- DN 55:7620
- OREF 55:1420b-d
- TI Use of the Wittig reaction for synthesis of  $\alpha,\beta$ -unsaturated and polyene acids
- AU Kucherov, V. F.; Kovalev, B. G.; Nazarova, I. I.; Yanovskaya, L. A.
- CS N. D. Zelinskii Inst. Org. Chem., Moscow
- SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1960) 1512-14 CODEN: IASKA6; ISSN: 0002-3353
- DT Journal
- LA Unavailable
- AB cf. W. and Haag, CA 50, 10030g. Refluxing 16.06 g. Ph3P:CHCO2Et with 2.64 g. cinnamaldehyde in C6H6 6 hrs. under N gave after treatment with petr. ether 2.85 g. Et 4-phenyl-1,3-butadienecarboxylate, 70.5%, b1 149-51°, n20D 1.5201; free acid m. 166-7°. Similarly were prepared: 48.5% EtCH:CHCO2Et, b17 54.5-5°, n21D 1.4310; 50% EtOCH2CH2CH:CHCO2Et, b7 73-6°, n19D 1.4427; 100% PhCH:CHCO2Et, b10 138-40°, n20D 1.5591; 50.6% (2-C4H3O)CH:CHCO2Et, b6 100°, n17D 1.5438; 67.5% Me2C:CH(CH2)2CMe:CHCH:CHCO2Et, b14 152-5°, n20D 1.5292; 34.1% CH2:CHCH:CHCO2Et, b19 60-1°, n21D 1.4819 (free acid m. 72°); 80.3% Me(CH:CH)2CO2Et, b8 71-2°, n21D 1.4940; 87% Me(CH:CH)3CO2Et, b0.3 61-3°, m. 39-40° (free acid m. 187-91°); 82% Me(CH:CH)4CO2Et, m. 90-3.5°; 88% Me(CH:CH)5CO2Et, m. 135-6°. Reaction with MeCHBrCHO gave 64.7% MeCHBrCH:CHCO2Et, b4 74-5°, n20D 1.4876. 2,4,6,8-Dodecatetraenecarboxylic acid, m. 226-7°, was prepared by saponification of the Et ester with aqueous MeOH solution of NaOH.

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E 2,4-PENTADIENEOIC ACID/CN
E 2,4-PENTADIENOIC ACID/CN
E 2,4-PENTADIENOIC ACID, 5-METHYL/CN
L2 STRUCTURE UPLOADED

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FILE 'REGISTRY' ENTERED AT 06:27:46 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:28:11 ON 11 DEC 2007

FILE 'REGISTRY' ENTERED AT 06:29:04 ON 11 DEC 2007 E 2,4-PENTADIENOIC ACID/CN

· L6 1 E3

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FILE 'REGISTRY' ENTERED AT 06:32:17 ON 11 DEC 2007

FILE 'CAPLUS' ENTERED AT 06:32:27 ON 11 DEC 2007 33 L6/PREP

FILE 'REGISTRY' ENTERED AT 06:38:10 ON 11 DEC 2007 E 5-PHENYL- 2,4-PENTADIENOIC ACID/CN E 2,4-PENTADIENOIC ACID, 5-PHENYL/CN

L9 2 E4

L8

FILE 'CAPLUS' ENTERED AT 06:39:43 ON 11 DEC 2007 10 158 L9

L10 158 L9
L11 0 9/THU
L12 10 L9/THU
L13 52 L9/PREP
L14 49 L13 NOT L12

=> d 114 17-27 ti

L14 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN

- TI Cinnamylideneacetic acid and its derivatives
- L14 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and triterpenes from Asclepias linaria
- L14 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Condensation of ethyl crotonate, 3-methylcrotonate, and isopropylidenemalonate with aromatic aldehydes
- L14 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis and NMR and IR spectra of  $\alpha$ -trans- $\gamma$ -cis- $\beta$ -styrylacrylic acid
- L14 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Condensation of 2-alkyl-substituted salts of 1,3-dioxolanium with aldehyde acetals. Synthesis of unsaturated aromatic and heterocyclic acids
- L14 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Polyhalogenated α,α'-diethylenic ketones. Synthesis and properties of polychlorinated 3-pentadienones and 3-heptatrienones
- L14 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis of cinnamylideneacetic acid by the Perkin reaction
- L14 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Use of sulfuric acid as a condensing reagent
- L14 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Ethyl esters of  $\alpha,\beta$ -unsaturated esters by the PO olefination method
- L14 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Reactions with phosphinealkylenes. VIII. Novel synthesis of carboxylic acids from phosphine alkylenes
- L14 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Isomerization of terphenyls
- => d 114 17-20 ti fbib abs
- L14 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Cinnamylideneacetic acid and its derivatives
- AN 1975:155832 CAPLUS
- DN 82:155832
- OREF 82:24856h,24857a
- TI Cinnamylideneacetic acid and its derivatives
- IN Tsuda, Minoru; Tanaka, Hideaki
- PA Agency of Industrial Sciences and Technology, Japan
- SO Jpn. Tokkyo Koho, 3 pp. CODEN: JAXXAD
- DT Patent
- LA Japanese
- FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	JP 49047735	В	19741217	JP 1969-20056 JP 1969-20056	19690318 19690318		

AB Reaction of 0.5 mole PhCH:CHCHO with 1.5 mole Ac2O over 0.5 mole AcOK at 40° gave 52% PhCH:CHCH:CHCO2H. The large excess of Ac2O inhibited polymerization of the aldehyde and product.

- L14 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and triterpenes from Asclepias linaria
- AN 1975:54218 CAPLUS
- DN 82:54218
- OREF 82:8659a,8662a
- TI  $\beta$ -Amyrin juarezate, a novel ester from Marsdenia pringlei and triterpenes from Asclepias linaria
- AU Dominguez, Xorge A.; Marroquin, Jorge; Olguin, Luz M.; Morales, Francisco; Valdez, Victoria
- CS Dep. Quim., Inst. Tecnol. Estud. Super. Monterrey, Monterrey, Mex.
- SO Phytochemistry (Elsevier) (1974), 13(11), 2617-18 CODEN: PYTCAS; ISSN: 0031-9422
- DT Journal
- LA English
- AB Exts. of M. pringlei, obtained by successive plant treatment with light petrol and EtOH were chromatographed over silica gel, and the chromatograms were eluted with solvents of increasing polarity, starting with C6H6 and proceeding to MeOH, the petrol extract yielding β-amyrin juarezate and the EtOH extract giving kondurite. On hyrogenation, β-amyrin 4-phenylvalerate was obtained. The petrol extract of A. linaria was sep. into individual constituents by a combination of column and preparative thin-layer chromatog. yielding triacontane, ψ-taraxasteryl acetate, sitosterol, and oleanolic acid.
- L14 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Condensation of ethyl crotonate, 3-methylcrotonate, and isopropylidenemalonate with aromatic aldehydes
- AN 1973:546113 CAPLUS
- DN 79:146113
- OREF 79:23681a,23684a
- TI Condensation of ethyl crotonate, 3-methylcrotonate, and isopropylidenemalonate with aromatic aldehydes
- AU Angelova, Iordanka; Ivanov, Chavdar
- CS Chem. Fac., Univ. Kl. Ohridsky, Sofia, Bulg.
- SO Chemische Berichte (1973), 106(8), 2643-7 CODEN: CHBEAM; ISSN: 0009-2940
- DT Journal
- LA German
- GI For diagram(s), see printed CA Issue.
- AB RC6H4CHO (R = H, 4-Me, 4-MeO, 2- or 4-Cl) reacted with H2NNa and MeCR1:CHCO2Et (Rl = H, Me) or Me2C:C(CO2Et)2 in DMF to give RC6H4CH:CHCR1:CHCO2H or the lactones (I), resp. I were formed via (RC6H4CH:CH)2C:C(CO2H)2.
- L14 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Synthesis and NMR and IR spectra of  $\alpha\text{-trans-}\gamma\text{-cis-}\beta\text{-styrylacrylic}$  acid
- AN 1973:418302 CAPLUS
- DN 79:18302
- OREF 79:2939a,2942a
- TI Synthesis and NMR and IR spectra of  $\alpha\text{-trans-}\gamma\text{-cis-}\beta\text{-styrylacrylic}$  acid
- AU Stepanova, O. S.; Galatina, A. I.; Nguyen Van Tong
- CS Odess. Univ., Odessa, USSR
- SO Voprosy Stereokhimii (1972), No. 2, 109-13 CODEN: VSTKB9; ISSN: 0372-6762
- DT Journal
- LA Russian
- AB PhC.tplbond.CCHO reacted with BrCH2CO2Me in the presence of Zn-C6H6 to give PhC.tplbond.CCH(OH)CH2CO2Me, which was dehydrated with POC13 to trans-PhC.tplbond.CCH:CHCO2Me (I). Selective hydrogenation of I, followed by hydrolysis, gave α-trans-γ-cis-PhCH:CHCO2H (II). The

# ir and NMR spectra of II were studied.

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STRUCTURE FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2 DICTIONARY FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> e 2.4.6-h	eptatr	ienoic acid, 5-phenyl/cn
E1	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E3		2,4,6-HEPTATRIENOIC ACID, 5-PHENYL/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
E5 .	ī	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL
Ц	-	ESTER/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
	_	, METHYL ESTER, (2Z,4Z)-/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
		7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
		7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
•		RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
		RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
		RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
		RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E,
		4E) -/CN
=> e e1	_	
E1	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-(6,7,7-TRIMETHYL-2,3-DI
		OXABICYCLO(2.2.2)OCT-5-EN-1-YL)-, METHYL ESTER, (E,E,E)-/CN
E2	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-(6,7,7-TRIMETHYL-2,3-DI
		OXABICYCLO(2.2.2)OCT-5-EN-1-YL)-, METHYL ESTER, (E,E,Z)-/CN
E3		2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E4	1	2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E5	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
E6	1	2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL
		ESTER/CN
E7	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
		, METHYL ESTER, (2Z,4Z)-/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
		7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
		7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
		RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
E11		2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
E11 E12	1	2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD

RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN

```
=> e 2,4,6-heptatrienoic acid, 5-phenyl-/cn
                  2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-/CN
E1
                   2,4,6-HEPTATRIENOIC ACID, 5-METHYL-7-PHENYL-, ETHYL ESTER/CN
E2
E3
             0 --> 2,4,6-HEPTATRIENOIC ACID, 5-PHENYL-/CN
E4
                   2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-, (E,E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6,7,7-TRICHLORO-3-HYDROXY-, ETHYL
             1
E.5
                   ESTER/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
E6
             1
                   , METHYL ESTER, (2Z,4Z)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
E7
             1
                   7-PHENYL-, METHYL ESTER, (2Z,4E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(((DIMETHYLAMINO)CARBONYL)THIO)-
             1
E8
                   7-PHENYL-, METHYL ESTER, (2Z,4Z)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
             1
E9
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, (2E,4E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
             1
E10
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
E11
             1
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
E12
             1
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E,
                    4E) -/CN
=> e e12
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
             1
E1
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-, METHYL ESTER, (2E,4E)-/CN
                   2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
             1
E2
                   RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, (2E,4E)-/CN
             1 --> 2,4,6-HEPTATRIENOIC ACID, 6-(6-(1,1-DIMETHYLETHYL)-2,3-DIHYD
E3
                    RO-1,1-DIMETHYL-1H-INDEN-4-YL)-3-METHYL-, METHYL ESTER, (2E,
                    4E) -/CN
             1
                    2,4,6-HEPTATRIENOIC ACID, 6-(ACETYLOXY)-7-PHENYL-, METHYL ES
E4
                    TER, (2Z, 4E) - /CN
                    2,4,6-HEPTATRIENOIC ACID, 6-(ACETYLOXY)-7-PHENYL-, METHYL ES
E5
             1
                    TER, (2Z, 4Z) - /CN
                    2,4,6-HEPTATRIENOIC ACID, 6-(DIMETHOXYPHOSPHINYL)-, METHYL E
             1
E6
                    STER, IRON COMPLEX, (E,E)-/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-(HYDROXYMETHYL)-, METHYL ESTER,
             1
E7
                    IRON COMPLEX, (E,E)-/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-FLUORO-3-METHYL-7-(1,2,3,4-TETRA
E8
             1
                    HYDRO-6-QUINOLINYL)-, (2E, 4E, 6E)-/CN
E9
             1
                    2,4,6-HEPTATRIENOIC ACID, 6-FORMYL-7-((2-(1H-INDOL-3-YL)ETHY
                    L) AMINO) -2- (METHYLTHIO) -, ETHYL ESTER/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-, METHYL ESTER/CN
E10
             1
                    2.4.6-HEPTATRIENOIC ACID, 6-METHYL-3-(TRIFLUOROMETHYL)-, ETH
             1
E11
                    YL ESTER, (2E, 4E) - /CN
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, ETHY
             1
E12
                    L ESTER/CN
=> e e12
              1
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-, METHYL ESTER/CN
E1
E2
             1
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-3-(TRIFLUOROMETHYL)-, ETH
                    YL ESTER, (2E, 4E)-/CN
             1 --> 2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, ETHY
E.3
                    L ESTER/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, METH
              1
E4
                    YL ESTER/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(1H-PYRROL-2-YL)-, METH
E5
              1
                    YL ESTER, (E, E, E) - /CN
             1
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(4-NITROPHENYL)-, ETHYL
E6
                     ESTER, (2E, 4E, 6E)-/CN
                    2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(5-NITRO-2-FURANYL)-, (
E7
              1
```

		E, E, E) -/CN
E8	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(5-NITRO-2-FURANYL)-, M
		ETHYL ESTER, (E,E,E)-/CN
E9	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3,4-DIHYDRO
		XY-2,4,5-TRIMETHYL-2-FURANYL)-, ETHYL ESTER, (2A(2E,4E
		,6E),3B,4A,5A)-/CN
E10	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3,4-DIHYDRO
		XY-2,4,5-TRIMETHYL-2-FURANYL)-, ETHYL ESTER, (2A(2E,4E
		$,6E),3B,4A,5A)-(\pm)-/CN$
E11	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3-HYDROXY-4
		-((2-METHOXYETHOXY)METHOXY)-2,4,5-TRIMETHYL-2-FURANYL)-, ETH
		YL ESTER, (2A(2E, 4E, 6E), 3B, 4A, 5A)-/CN
E12	1	2,4,6-HEPTATRIENOIC ACID, 6-METHYL-7-(TETRAHYDRO-3-HYDROXY-4
		-((2-METHOXYETHOXY)METHOXY)-2,4,5-TRIMETHYL-2-FURANYL)-, ETH
		YL ESTER, (2A(2E, 4E, 6E), 3B, 4A, 5A)-(.+
		) -/CN

=> logoff hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.70	253.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:38:44 ON 11 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

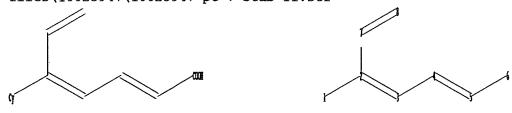
# PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* \* SESSION RESUMED IN FILE 'REGISTRY' AT 07:46:43 ON 11 DEC 2007 FILE 'REGISTRY' ENTERED AT 07:46:43 ON 11 DEC 2007 COPYRIGHT (C) 2007 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.70	253.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10025947\10025947 pt V stab II.str



chain nodes :

1 2 3 4 5 6 7 8

chain bonds:

1-2 2-3 2-7 3-4 4-5 5-6 7-8

exact/norm bonds:

1-2

exact bonds:

2-3 2-7 3-4 4-5 5-6 7-8

Match level:

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

# L16 STRUCTURE UPLOADED

=> d 116 L16 HAS NO ANSWERS L16 STR

Structure attributes must be viewed using STN Express query preparation.

=> search 116 sss sam
SAMPLE SEARCH INITIATED 07:47:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 484 TO ITERATE

100.0% PROCESSED 484 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8361 TO 10999
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> search 116 sss full FULL SEARCH INITIATED 07:47:20 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 9406 TO ITERATE

100.0% PROCESSED 9406 ITERATIONS 3 ANSWERS SEARCH TIME: 00.00.01

L18 3 SEA SSS FUL L16

=> d mscan
'MSCAN' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN

SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data

IDE - FIDE, but only 50 names SQIDE - IDE, plus sequence data

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQD - Protein sequence data, includes RN

SQD3 - Same as SQD, but 3-letter amino acid codes are used

SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

APPS -- Application and Priority Information

BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number

CBIB -- CA Accession Number, plus Bibliographic Data (compressed)

IND -- Index Data

IPC -- International Patent Classification

PATS -- PI, SO

STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels

IBIB -- BIB, indented, with text labels

ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields. HELP FORMATS -- To see detailed descriptions of the predefined formats. ENTER DISPLAY FORMAT (IDE):end

=> d scan

L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2,4,6-Heptatrienoic acid, 7-(2,3,6,7,9,12-hexahydro-2,2,7,7-tetramethyl-9oxo-1H,5H-pyrido[3,2,1-gh][1,7]phenanthrolin-10-yl)-5-phenyl-

MF C32 H34 N2 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C15 H11 N O6

$$\begin{array}{c|c} CH = CH_2 & CO_2H \\ \hline O_2N & C = CH - CH = C \end{array}$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L18 3 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 2,4,6-Heptatrienoic acid, 7-(12-ethyl-2,3,6,7,11,12-hexahydro-2,2,7,7tetramethyl-11-oxo-1H,5H-pyrido[3,2,1-gh][1,7]phenanthrolin-10-yl)-5phenyl-

MF C34 H38 N2 O3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

176.60 426.92 FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION -17.94CA SUBSCRIBER PRICE 0.00

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 07:49:33 ON 11 DEC 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

#### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \* SESSION RESUMED IN FILE 'REGISTRY' AT 08:53:05 ON 11 DEC 2007 FILE 'REGISTRY' ENTERED AT 08:53:05 ON 11 DEC 2007 COPYRIGHT (C) 2007 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	176.60	426.92
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.94

```
=> e 2,4-pentadienoic acid, 5,5-diphenyl-/cn
                 2,4-PENTADIENOIC ACID, 5,5-DIHYDROXY-3-ISOPROPYL-, LACTONE/C
                  2,4-PENTADIENOIC ACID, 5,5-DIHYDROXY-3-METHYL-2-PROPIONYL-,
E2
             1
                   Δ-LACTONE/CN
             1 --> 2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-/CN
F.3
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (2E)-/CN
E4
             1
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (E)-/CN
E5
             1
                   2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, (Z)-/CN
E6
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, 4-NITROPHENYL ESTER, (
E7
             1
                  E) -/CN
E.S
            1
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER/CN
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (2E)-/CN
E9
            1
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (2Z)-/CN
E10
            1
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (E)-/CN
E11
            1
                  2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-, ETHYL ESTER, (Z)-/CN
            1
E12
```

=> e3

1 "2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-"/CN L19

=> d 119

L19 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

19625-92-4 REGISTRY

Entered STN: 16 Nov 1984 ED

2,4-Pentadienoic acid, 5,5-diphenyl- (6CI, 8CI, 9CI) (CA INDEX CN NAME)

MF C17 H14 O2

STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, USPAT2, USPATFULL LC (\*File contains numerically searchable property data)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file reg

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
184.40
434.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -17.94

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STRUCTURE FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2 DICTIONARY FILE UPDATES: 10 DEC 2007 HIGHEST RN 957336-90-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> 119

L20 1 "2,4-PENTADIENOIC ACID, 5,5-DIPHENYL-"/CN

=> d 120

- L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 19625-92-4 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN 2,4-Pentadienoic acid, 5,5-diphenyl- (6CI, 8CI, 9CI) (CA INDEX NAME)
- MF C17 H14 O2
- LC STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, USPAT2, USPATFULL (\*File contains numerically searchable property data)

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 7.35 442.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL

ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -17.94

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- L21 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Preparation of benzofuran moiety-containing piperazine derivatives as inhibitors of STAT-6 phosphorylation
- AN 2002:521719 CAPLUS
- DN 137:93769
- TI Preparation of benzofuran moiety-containing piperazine derivatives as inhibitors of STAT-6 phosphorylation
- IN Kawakatsu, Nobuyuki; Namiki, Takayuki; Yamazaki, Norihisa; Yuasa, Masayuki; Miki, Toyohiko; Suenobu, Noriko; Shimanuki, Tomomasa
- PA Pola Chemical Industries, Inc., Japan
- SO PCT Int. Appl., 33 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

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The title compds. I [Al = (CHR1)a; A2 = (CH:CH)q; A3 = (CH2)m; B1 = (CH2)n; B2 = (CR2R3)b; B3 = (CH2)p; R1 is Ph or hydrogen; a is 0 or 1; m, n, b, p, and q are each independently an integer of 0 to 5; and R2 and R3 are each independently hydrogen or hydroxyl, or alternatively R2 and R3 together represent oxygen; a proviso is given] are prepared I inhibit the phosphorylation of STAT 6 and are useful in the treatment or prevention of allergy. The activity of compds. of this invention against JAK-STAT-6 phosphorylation was demonstrated. A formulation is given.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
TI 5,5-Diarylpenta-2,4-dienoic acid amides as potential antimalarial agents
AN 1968:426954 CAPLUS
DN 69:26954
OREF 69:5003a,5006a

- TI 5,5-Diarylpenta-2,4-dienoic acid amides as potential antimalarial agents
- AU Colwell, William T.; Lange, Judy H.; Henry, David W.
- CS Stanford Res. Inst., Menlo Park, CA, USA
- SO Journal of Medicinal Chemistry (1968), 11, 749-52 CODEN: JMCMAR; ISSN: 0022-2623
- DT Journal
- LA English
- GI For diagram(s), see printed CA Issue.
- AB A series of 5,5-diaryl-penta-2,4-dienoic acids and their amides were synthesized and evaluated as antimalarial agents. The acids were prepared from the corresponding diaryl ketones either directly by a Reformatskii procedure or through acetylenic alc. and acrolein intermediates. The preparation of a series of 3,3-bis(4-chlorophenyl)-acrylamides is also reported. One compound, N,N-diethyl-5,5-bis(4-chlorophenyl)penta-2,4-dienoic acid amide (I), provided significant antiplasmodial activity.
- L21 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
- TI Reformatskii reaction in syntheses of  $\omega, \omega$ -diarylalkanoic acids and related compounds
- AN 1959:44983 CAPLUS
- DN 53:44983
- OREF 53:8063b-i,8064a-i
- TI Reformatskii reaction in syntheses of  $\omega, \omega$ -diarylalkanoic acids and related compounds
- AU Klemm, L. H.; Bower, G. M.
- CS Univ. of Oregon, Eugene
- SO Journal of Organic Chemistry (1958), 23, 344-8 CODEN: JOCEAH; ISSN: 0022-3263
- DT Journal
- LA Unavailable
- OS CASREACT 53:44983
- Ph2CO and various MeO-substituted benzophenones were submitted to the AΒ Reformatskii reaction with BrCH2CO2Et (I) and BrCH2CH:CHCO2Me (II), and an attempt made to correlate the data obtained with others quoted in the literature. Following the general procedure of Gardner (C.A. 49, 12358c) 57 g. p-MeOC6H4CO2H and 41 g. MeOPh stirred 2 hrs. at  $70^{\circ}$  with 540g. polyphosphoric acid, the mixture poured into ice H2O, the precipitate washed with 500 ml. 5% aqueous NaOH and with H2O, and the dried product crystallized (alc.) yielded 75-4, g. (p-MeOC6H4)2CO (III), m. 144-6°. Similarly 41 g. 3,4,5-(MeO) 3C6H2CO2H, 25 g. 1,2-(MeO) 2C6H4, and 430 g. polyphosphoric acid gave 36 g. 3,3',4,4',5-pentamethoxybenzophenone (IV). Zn (50 g., 20-mesh activated with HCl), 58.3 g. III, and a crystal of iodine in 400 ml. anhydrous C6H6 stirred under reflux with addition of 70 g. I in 20 ml. C6H6, the mixture refluxed 15 min. and diluted with 200 ml. 10% AcOH, the aqueous layer extracted with C6H6, the combined organic solns. washed (H2O,

excess 1.5% NH4OH, H2O), dried (MgSO4), and evaporated gave 55 g.
RR'C(OH)CH2CO2Et (V, R = R' = p-MeOC6H4) (VI), m. 92-3° (EtOAc).
VI (14.4 g.) in 140 ml. warm dry C6H6 and 20 ml. anhydrous HCO2H refluxed 5 min., the C6H6 removed in a current of air, the residual unsatd. ester hydrogenated 30 min. in 90 ml. AcOH at 3.5-4.0 atmospheric with 2.5 g. 5% Pd-C, the filtered solution evaporated, and the residue crystallized yielded 83% RR'CHCH2CO2Et (VII, R = R' = p-MeOC6H4) (VIII), m. 49.5-50.5° (absolute alc.), hydrolyzed 1 hr. by refluxing with 3% KOH in 75% alc., the concentrated solution acidified with HCl, and the precipitate recrystd. (absolute alc.) to give 97%

RR'CHCH2CO2H (IX, R = R' = p-MeOC6H4) (X), m. 138.5-9.5°. Similar hydrolysis of the residual unsatd. ester (from dehydration of 5 g. VI) yielded 4.1 g. (p-MeOC6H4)2C:CHCO2H, m. 146.5-7.5° (dilute MeOH). IV and 3-MeOC6H4Bz were similarly treated in refluxing C6H6 with I. The % yields for various methoxy-substituted benzophenones in the Reformatskii reaction with I were tabulated for comparison (position of substituents, % yield of V, and over-all % yield of IX given): none, 95, -; 2, 60-70, -;

3, 95-100, 88; 4, 78, 67; 4, 4', 69, 56; 3, 3', 4, 4', 81, -; 3, 4, 4', 5, 70, -; 3, 3', 4, 4', 5, -, 59. From these results it was anticipated that diaryl ketones would react readily with II but with lower yields due to an increasing number of possible side reactions. Zn (4.4 g., activated 20-mesh), 20 g. Ph2CO, 55 ml. dry C6H6, 35 ml. anhydrous Et2O, and a crystal of iodine treated in 1 hr. with 10 g. II in 25 ml. C6H6, the mixture stirred and refluxed 2 hrs. with 2 g. Zn, and treated with 45 ml. 2N AcOH, the organic layer washed (5% aqueous NaHCO3 and H2O), dried (Na2SO4) and evaporated, the

residual oil warmed 15 min. with 2 vols. anhydrous HCO2H, the mixture evaporated in

the

a current of air, and the residue fractionally distilled gave 32% Ph2C: CHCH: CHCO2Me (XI), m. 86-7° (MeOH), refluxed 2 hrs. with a slight excess of 2% KOH in MeOH and the solution acidified to give a quant. yield of Ph2C: CHCH: CHCO2H, m. 190-1° (PhMe). XI (15 g.) in 150 ml. AcOH hydrogenated 10 min. at 3.5-4.0 atmospheric with 3 g. 5% Pd-C and the filtered solution distilled gave 97% colorless Ph2CH(CH2)3CO2Me, b0.5 145-50°, hydrolyzed to yield quantitatively Ph2CH(CH2)3CO2H, m. 92.5-3.5° (60% alc.), converted by SOC12 to the corresponding Ph2CH(CH2)3COC1 (XII). XII (from 10 q. acid and 8 ml. SOCl2) in 250 ml. purified CS2 added through the Leonard and Sentz attachment (C.A. 48,676d) in 10 hrs. with stirring and refluxing to 2.7 g. anhydrous AlCl3 in 750 ml. CS2 with addns. of 2.7 g. AlC13 at 3-hr. intervals, the mixture stirred 2 hrs. and diluted with H2O, the organic layer from the filtered mixture distilled and the residue taken up in C6H6, the washed (excess 10% aqueous K2CO3 and H2O), dried (MgSO4) solution evaporated, and the residue distilled at 190-200°/0.5 mm. yielded 5.47 g. 9-phenyl-5-benzosuberone (XIII), m. 71.0-1.5° (dilute alc.); oxime, m. 152.5-3.5° (C6H6-petr. ether). XIII (2 g.) submitted to Huang-Minlon-Wolff-Kishner reduction, the diluted mixture extracted with C6H6,

H2O-washed and dried (MgSO4) extract distilled, and the liquid (1.2 g., bl.0 132-5°) redistd. gave 5-phenylbenzosuberan (XIV), b2 149-50°, m. 41-5°. PhMgBr (0.4 g. Mg, 2.4 g. PhBr, 75 ml. Et2O) treated slowly at 0° (ice-bath) with 2 g. 5-benzosuberone (obtained by cyclization of PhCH2(CH2)3CO2H with polyphosphoric acid) in 20 ml. Et2O, the mixture stirred 30 min. at 0° and refluxed 1 hr., the mixture hydrolyzed and the carbinol dehydrated with HCO2H according to Klemm and Ziffer (C.A. 50, 4094f), the product distilled at 1.5 mm. to give 0.4 g. colorless ketonic liquid (presumably starting material) and 1 g. KMnO4-reducing liquid. bl.5 115-35°, the alkenic fraction (0.9 g.) in 25 ml. AcOH hydrogenated 2 hrs. at 4 atmospheric with 0.1 g. prereduced PtO2.

and the filtered solution distilled yielded 0.56 g. XIV, b2 149-50°,  $\lambda$  3.26-3.52, 6.24, 6.71, 6.90, 13.35, 13.9, 14.35  $\mu$ . XIII (2.36 g.), 1.48 g. HCO2Et, and a few ml. C6H6 stirred and warmed with 0.5 g. NaH (N atmospheric), the red paste stirred 1.5 hrs. at 50° in 10 ml. C6H6 and treated successively with 3 ml. AcOH and 30 ml. H2O, the H2O-washed C6H6 layer extracted with 100 ml. 10% aqueous Na2CO3, the alkaline extract acidified, and the

precipitate recrystd. (EtOAc) gave material, m. 101.5-2.5°, repeatedly recrystd. (C6H6-ligroine) to give 6-hydroxymethylene-9-phenyl-5-benzosuberone, m. 102.0-2.5°. Attempts to apply the same conditions as used for Reformatskii reaction of II with Ph2CO to the reaction of II with the methoxy-substituted benzophenones found to condense readily with I gave only very small quantities of crude resinous products. An alternate pathway to the preparation of diarylvaleric acids was investigated starting with VIII, prepared by the Reformatskii reaction of III with I. LiAlH4 (3.3 g.) in 400 ml. anhydrous Et2O stirred with addition of 29 g. VIII in 110 ml. Et2O at a rate to maintain gentle refluxing, the mixture refluxed 1 hr., treated cautiously with EtOAc and 200 ml. cold 3N HCl, the aqueous phase extracted with 150 ml. Et2, the combined Et2O solns.

(H2O), dried (MgSO4) and evaporated, the viscous residue taken up in Et2O, and

the solution kept at -5° gave 85% (p-MeOC6H4)2CH(CH2)2OH (XV), m. 54-5° (Et2O); 3,5-dinitrobenzoate, m. 116-17° (C6H6-ligroine). XV (55 g.) in 250 ml. CCl4 at -5° stirred with addition in 2 min. of 27 g. freshly distilled PBr3, the mixture stirred 30 min. and the solution kept at room temperature overnight, warmed 20 min. at 50° and diluted with H2O, the aqueous phase extracted with CCl4, the combined CCl4 solns. washed repeatedly with H2O, the dried solution (CaCl2) evaporated and

the

residue in 200 ml. absolute alc. distilled azeotropically with 20 ml. dry C6H6 until the distilling temperature reached 78°, the solution refluxed 5 hrs. with NaCH(CO2Et)2 (from 4.6 g. Na, 350 ml. absolute alc., 32 g. H2C(CO2Et)2), the decanted liquid refluxed 2 hrs. with 28 g. KOH in 100 ml. H2O, the mixture concentrated, diluted with H2O, washed with Et2O and acidified, the crystalline product

distilled at 240-70°/1 mm., and the distillate crystallized (EtOAc) gave 31% (p-MeOC6H4)2CH(CH2)3CO2H, m. 103.5-4.0°. By the same procedures as used with III, 15 g. Zn, 25 g. IV, and 15 g. I gave V [R = 3,4-(MeO) 2 C6H3, R' = 3,4,5-(MeO) 3C6H2], dehydrated with 50 ml. anhydrous HCO2H and the resultant yellow liquid hydrogenated in 200 ml. AcOH with 2 g. 30% Pd-C to give 18 g. VII [R = 3,4-(MeO) 2C6H3, R' =3,4,5-(MeO)3C6H2], m. 81.5-82.5° (absolute alc.), hydrolyzed and the product purified by 2 recrystns. (C6H6-C6H14) and drying 12 hrs. at  $80^{\circ}/1$  mm. to give the acid IX [R = 3,4-(MeO)2C6H3, R' = 3,4,5-(MeO)3C6H2]. Similarly 15 g. Zn, 21.2 g. p-MeOC6H4Bz and 25 g. I gave 78% V (R = Ph, R' = p-MeOC6H4), m.  $79-80\degree$  (EtOAc), converted by dehydration, hydrogenation, and hydrolysis to yield 86% IX (R = Ph, R' = p-MeOC6H4), m.  $120-2^{\circ}$ . Repetition of the same transformations on 8.5 g. 3-MeOC6H4Bz produced 9.1 g. crude yellow acid, m. 92-8°, recrystd. (EtOAc-petr. ether) to give IX (R = Ph, R' = m-MeOC6H4), m. 99-100°. Following the general procedure of Huang-Minlon (C.A. 41, 1649a), 10 g. BzCH2(CH2)2CO2H, 7.5 g. NaOH, 7.5 ml. 95% N2H4, and 80 ml. (HOCH2CH2) 20 gave 8.4 g. PhCH2 (CH2) 3CO2H, m. 56.6-7.5° (Et20-petr. ether), identical with the product obtained by Clemmensen reduction of the

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